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Nomenclature of Organic Chemistry. IUPAC Recommendations and Preferred Names 2013.

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School of Biological and Chemical Sciences, Queen Mary University of London,
Mile End Road, London, E1 4NS, UK

Prepared by Dr G P Moss <g.p.moss@qmul.ac.uk>

All noted corrections have been incorporated in this version. Otherwise the text is as close to the printed book as possible.

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† Deceased

PREFACE

This edition of the *Nomenclature of Organic Chemistry* follows the 1993 publication of the *Guide to IUPAC Nomenclature of Organic Compounds* by the International Union of Pure and Applied Chemistry (IUPAC). The International Union of Pure and Applied Chemistry has the responsibility to establish rules for systematic nomenclature. The Rules for Organic Chemistry were first issued in Geneva in 1892. They were followed by the Liége Rules in 1930 and the IUPAC rules in 1957 (Sections A and B), 1969 (Sections A, B, and C) codified as the Blue Book, and 1979 (Sections A, B, C, D, E, F, and H). The 1993 Guide recognized the necessity to propose to the chemical community the so called 'preferred IUPAC name', not to say the 'unique name'. The explosion of information justifies this new approach in the revision of the principles, rules, and conventions of the nomenclature of organic compounds. Preferred IUPAC names, known under the friendly acronym PIN, are also important in legal situations, with manifestations in patents, export-import regulations, health and safety information, and communications in environmental sciences and their legal implications.

The work for this edition began in 1992 at the time the 1993 Guide was in press under the expert guidance of the Commission on Nomenclature of Organic Chemistry (CNOC). The general format of the Guide was maintained. The principal objective was to maintain continuity and consistency. Continuity meant that substitutive nomenclature was maintained as the principal nomenclature to name organic compounds based on the concepts of parent hydrides and of different hierarchical orders: order of classes, order of seniority of suffixes, seniority order for rings and ring systems, and seniority order for chains (the principal chain). Consistency was to consider the hydrides of elements of Groups 13, 14, 15, 16, and 17 as parent hydrides in substitutive nomenclature and to treat equally carbon atoms and heteroatoms. To achieve this goal, the names of the hydrides of heteroatoms are names ending in 'ane', for example 'phosphane' for PH_3 and 'silane' for SiH_4. As they are chosen amongst several (inorganic) names, for instance 'sulfane' and 'hydrogen sulfide' for H_2S, these names are called 'preselected names'; the decision to accept them as 'preferred IUPAC names' will be made later. Preselected names generate preselected prefixes and suffixes, for example 'sulfanyl' and 'sulfanylidene' for –SH and =S, respectively, which are used in substitutive nomenclature, as are preferred prefixes and suffixes, such as 'methyl', $–CH_3$, and 'phenyl', $–C_6H_5$.

Several changes from previous rules were needed to achieve systematization and consistency in constructing names. To facilitate the understanding and use of the preferred IUPAC name system, these changes are explained and highlighted in boxes each and every time they appear in Chapters P-1 through P-8. In Chapter P-6, full systematization has been applied to the formation of prefixes of substituent and functional groups.

It is hoped that the systematization provided by the strict application of the rules will be widely understood and accepted. Preferred IUPAC names are easy to be selected. It is however inevitable that some ambiguities and unsuspected difficulties will be encountered. Task forces will be established to rapidly answer questions, give guidance to authors and ensure the homogeneity of the system. Computerized nomenclature should help in maintaining this homogeneity and in making sure that further progress will be firmly consistent with it.

It is important to reiterate that nomenclature is here to serve a number of purposes: oral communication, commercial and industrial development, written scientific communication, etc. As has been many times, the prime aim of IUPAC nomenclature is clarity and the construction of unambiguous names; there must be absolute correspondence between structure and name, and vice versa between name and structure. Preferred IUPAC names are here today to serve a special purpose; they are not imposed to the chemical and scientific community. The rules set out here express the firm belief of the former Commission on Nomenclature for Organic Chemistry, now that of the IUPAC Chemical Nomenclature and Structure Representation Division, as to the best system of nomenclature, for present specific purposes and for future developments.

ACKNOWLEDGMENTS

Many thanks are due to a large number of contributors. The shaping of the project and supervision over the early draft stages was done by members of the IUPAC Commission on Nomenclature of Organic Chemistry from 1993 until it demise in 2001. The membership of the Commission on Nomenclature of Organic Chemistry from 1993 through 2001 is given above. In 2002, responsibility for the project then passed to the IUPAC Division of Chemical Nomenclature and Structure Representation who followed its development through 2013. The membership of the Division Committee from 2002 through 2013 is also given above. It is also in order to thank all members of the Division Committee and other colleagues who submitted general or specific comments and/or participated in discussions, either by correspondence, or by means of the IUPAC Division VIII Webboard located on the RSC web site during the preparation of the first full draft in 2004 on which many comments and suggestions were received. Many sincere thanks must be given to Alan McNaught who, along with the authors, spent many days reviewing the hundreds of comments and suggestions received on the 2004 draft which resulted in a revised draft in 2010 which was again posted for review on the Division VIII Webboard. Many comments made on the 2010 draft were simply repeats of the comments made for the 2004 draft. Significant and useful comments came from Jonathan Brecher, Ursula Bünzli-Trepp, Ture Damhus, Ted Godly, Harry Gotlieb, Richard Hartshorn, Karl-Heinz Hellwich, Bernardo Herold, J. Kahovec, L. Maat, Paulina Mata, József Nyitrai, Arhur Maximenko, Andrey Yerin, Richard Cammack, Hal Dixon, Gernot Eller, Rita Hoyos de Rossi, Jan Reedijk, Alexander Senning, L. Salvatella, Roger Sayle, and Hervé Schepers leading finally to these 2013 recommendations. We must also thank Marcus Ennis who spent weeks giving the 2013 draft a complete edit for errors in both language and chemistry.

CHANGES FROM THE 1979 EDITION, THE 1993 GUIDE, AND OFFICIAL PUBLICATIONS FROM 1993 THROUGH 2002 INCLUDED IN THE 2013 EDITION OF THE IUPAC *NOMENCLATURE OF ORGANIC CHEMISTRY, 2013 EDITION*

1. Scope of the recommendations in the 2013 edition

(a) The elements Al, Ga, In, and Tl are added to the elements that were included in the recommendations in the 1979 edition (ref. 1) and the 1993 Guide (ref. 2)

2. Skeletal replacement (‘a’) nomenclature

(a) Heteroatoms in chains subject to skeletal replacement (‘a’) nomenclature are considered to be an integral part of the parent hydride and as nondetachable prefixes they have seniority over suffixes for numbering; thus, heteroacyclic chains subject to skeletal replacement (‘a’) nomenclature are now treated the same as heterocyclic rings.

(b) The heteroatoms P, As, Sb, Bi, Si, Ge, Sn, Pb, B, Al, Ga, In, and Tl can now terminate a heteroacyclic chain that is subject to skeletal replacement (‘a’) nomenclature; in previous recommendations, a heteroacyclic chain that is subject to skeletal replacement (‘a’) nomenclature had to terminate with carbon atoms.

(c) Skeletal replacement (‘a’) prefixes ending in ‘ata’, for example ‘borata’, are no longer recognized.

(d) Groups of heteroatoms having a single multivalent name are considered as a unit; hence the term ‘heterounit’ includes both heteroatoms and such heteroatom groups. Such heteroatom groups were not considered as a single heterounit in previous recommendations.

(e) Adapting skeletal replacement (‘a’) prefixes for elements of Groups 1-12 for use in skeletal replacement nomenclature is a major change even though names for such organometallic compounds involving these elements are only preselected at this time.

3. Substitutive nomenclature

(a) Substitutive nomenclature is the preferred method of nomenclature, except for anhydrides, esters and salts, acid halides, and pseudohalides for which traditional functional class names are maintained. Substitutive nomenclature is based on the names of parent hydrides modified by suffixes and prefixes. Parent hydride names can be modified by using skeletal replacement (‘a’) nomenclature and functional replacement nomenclature, and also by additive operations (for example, addition of hydrogen atoms or ions) and subtractive operations (for example, subtraction of hydrogen atoms or ions).

(b) Generalized ‘ane’ nomenclature is recommended for preferred IUPAC names. Substitutive nomenclature is applied to each element of Groups 13, 14, 15, 16, and 17 having a fixed number of hydrogen atoms which are used as mononuclear or polynuclear parent hydrides in the same way as described for alkanes. Recommended names are ‘alumane’ for AlH_3, ‘gallane’ for GaH_3, ‘indigane’ for InH_3, and ‘thallane’ for TlH_3. Suffixes and prefixes are attached in the same way as for alkanes, for example ‘trisulfanecarboxylic acid’ for HSSS-COOH, ‘trimethylsilanol’ for $(CH_3)_3Si$-OH, ‘phenylstibanone’ for $C_6H_5Sb{=}O$, and trimethylalumane for $(CH_3)_3Al$.

(c) Some well entrenched and widely used trivial names are maintained to identify the parent hydrides: ‘methane’, ‘ethane’, ‘propane’ and ‘butane’ for alkanes and names of monocyclic and polycyclic carbocycles and heterocycles used to create all polycyclic fused rings. The number of retained names for functional parents and characteristic groups has been reduced, as has been done with each succeeding edition of the IUPAC ‘‘Nomenclature of Organic Chemistry’’.

(d) Toluene and xylene are retained preferred IUPAC names, but are not freely substitutable. Toluene is substitutable under certain conditions only in general nomenclature. Mesitylene is a retained name but only for general nomenclature and cannot be substituted. In the 1993 Guide (ref. 2), these parent hydrides were also retained but only limited substitution was allowed.

(e) Hydrazidines are named systematically as ‘-hydrazonohydrazides’ and not as hydrazones of the corresponding hydrazides as in the 1979 recommendations.

(f) Oximes are named substitutively as ‘*N*-hydroxy’ derivatives of imines and not by functional class nomenclature as in previous recommendations.

(g) Hydrazones and azines are named substitutively as ‘ylidene’ derivatives of hydrazine and not by functional class nomenclature as in previous recommendations.

4. Multiplicative nomenclature

(a) Multiplicative nomenclature is now extended to cyclic structures with or without characteristic groups; chains composed only of carbon atoms continue to be excluded. In past recommendations multiplicative nomenclature was limited to compounds having characteristic groups expressed as suffixes or implied by a retained name and to heterocyclic parent hydrides. The system now has also been expanded to allow substitution on the central unit of a multiplying group and the use of nonsymmetrical central units under specific conditions.

(b) In these recommendations, all substituent groups, including the principal characteristic groups must be identical and have the same locant in order to construct a multiplicative name. This is a change from earlier recommendations where such locants did not need to be identical.

5. Hydro or dehydro prefixes are introduced in names by an additive or subtractive operation and are now classified as detachable prefixes but are not included in the category of alphabetized detachable prefixes which describe substitution. In names, they occupy a permanent place between the nondetachable prefixes attached just before the parent structure and the alphabetizable detachable prefixes describing substitution. The change from nondetachable to nonalphabetizable detachable prefixes gives ‘hydro’ and ‘dehydro’ prefixes the same status with respect to numbering nomenclatural features in the construction of names as the subtraction of hydrogen atoms denoted by ‘ene’ and ‘yne’ endings. In names, the prefix ‘dehydro’ precedes the prefix ‘hydro’, when both are present. Simple numerical terms, such as ‘di-’,‘tetra-’, etc., are used with ‘hydro’ and ‘dehydro’ prefixes. Hydro or dehydro prefixes are numbered according to the principle of lowest locants, in accord with the numbering of the parent hydride and after priority has been given to indicated hydrogen, added indicated hydrogen, and suffixes, when present, as specified in the general rules for numbering.

6. Suffixes

(a) The suffix ‘peroxol’, for –OOH, has been added to the list of basic suffixes and is modified by functional replacement nomenclature, generating the suffixes ‘–*OS*-thioperoxol’ for –OSH, and ‘–*SO*-thioperoxol’ for –SOH. The suffix ‘sulfenic acid’, for –SOH, was abandoned in the 1993 Recommendations.

(b) Systematic suffixes, for example methanimidic acid, imidic acids, hydrazonic acids, peroxycarboxylic acids, and chalcogen analogues of monocarboxylic acids, are changes for formic acid, acetic acid, benzoic acid, and oxalic acid.

(c) Suffixes are now used in accordance with the seniority of classes (see P-41) for germanium, tin and lead compounds which is a change from the previous recommendations where only prefixes were used.

(d) The suffix '-hydrazide' rather than '-ohydrazide' used in previous recommendations is used for naming acyclic hydrazides in accordance with the general use of suffixes added to names of parent hydrides, for example pentanehydrazide for CH_3-CH_2-CH_2-CH_2-CO-NH-NH_2, not pentanohydrazide.

7. Prefixes

(a) The preselected prefix 'nitrilo' is used only when the three bonds from nitrogen are attached to different atoms; it is no longer used for the structure –N=, which now has the preselected prefix 'azanylylidene'.

(b) The preselected prefix 'azanediyl' derived from the preselected parent hydride name 'azane' is now used for the multiplicative substituent group –NH– ; the preselected prefix 'imino' is used only to designate =NH as a substituent.

(c) Prefixes derived from borane are now named only by the general method [method (2) in P-29.2], namely 'boranyl', 'boranylidene', and 'boranylidyne', rather than by the method used for the elements of Group 4 [method (1) in P-29.2]; the prefix 'boryl' is discarded.

(d) The preselected prefixes 'sulfanylidene', 'selanylidene', and 'tellanylidene', for =S, =Se, and =Te as substituents, respectively, are used in preferred IUPAC names to designate the chalcogen analogues of the preselected prefix 'oxo'. The prefixes 'thioxo', 'selenoxo', and 'telluroxo' derived by functional replacement nomenclature may be used in general nomenclature.

(e) Simple substitutive acyl prefixes directly derived from the name of a 'sulfonic acid', 'sulfinic acid', and their chalcogen analogues as in 'benzenesulfonyl' and 'benzenetellurodithioyl' are used in preferred IUPAC names and not prefixes formed by concatenation, for example 'phenylsulfonyl', which can be used in general nomenclature.

(f) The prefixes 'ureido' and 'ureylene' are not used in IUPAC names. The prefixes 'carbamoylamino' and 'carbonylbis(azanediyl)', respectively, are recommended for preferred IUPAC names and in general nomenclature.

(g) The prefix 'guanidino' is no longer acceptable in preferred IUPAC names but may be used in general nomenclature; the preferred prefix is 'carbamimidoylamino'.

(h) The prefix 'amidino' is no longer acceptable in IUPAC names; the preferred prefix is 'carbamimidoyl'.

(i) The prefix '*aci*-nitro' for HO-N(O)= is no longer acceptable for preferred IUPAC names; it was discontinued in the 1993 Guide (ref. 2). The preferred prefix is 'hydroxy(oxo)-λ^5-azanylidene'; the prefix recommended in the 1993 Guide (ref. 2) 'hydroxynitroryl' is not acceptable in the context of these recommendations where two free valences must be expressed by the correct 'ylidene' or 'diyl' type.

(j) Preselected prefixes derived from the preselected parent hydride hydrazine are now formed systematically from hydrazine: 'hydrazinyl' for H_2N-NH– ; 'hydrazinylidene' for H_2N-N=; 'hydrazinediylidene' for =N-N=; and hydrazine-1,2-diyl for –NH-NH–. The prefixes 'hydrazino', 'hydrazono', 'azino' and 'hydrazo', respectively, are no longer acceptable, even for general nomenclature.

(k) The prefixes 'benzyl', 'benzylidene', and 'benzylidyne' cannot be substituted for preferred IUPAC names, although for general nomenclature restricted substitution is permitted (see P-29.6.2). In the 1993 Guide (ref. 2), these prefixes could only be substituted on the ring.

(l) Preferred prefixes derived from 'triazane' and 'tetraazane' are named systematically as hydrocarbons are named, for example 'triazan-1-yl', 'tetraazan- 2-yl'. The prefixes 'triazano' and 'tetraazano' previously used for 'triazan-1-yl' and 'tetraazan-1-yl' and also as bridge prefixes must not be used even though as bridge prefixes they are now named 'epitriazano', etc.

(m) Acyl prefixes formed from acyclic parent hydrocarbons and prefixes such as 'oxo', 'thioxo', 'sulfanylidene', and 'imino', for example, '1-oxopropyl' are not preferred prefixes for preferred IUPAC names, but can be used in general nomenclature; they are used in CAS index nomenclature.

(n) Functional replacement analogues of formic, acetic, benzoic, and oxalic acids and acyl prefixes derived from them are named systematically, for example, methanimidic acid not formimidic acid, benzenecarboximidoyl not benzimidoyl, and ethanediperoxoic acid not diperoxyoxalic acid.

(o) Simple prefixes are used before prefixes beginning with a multiplicative prefix where 'bis-','tris-', etc., were used in previous recommendations.

(p) The –N=C=O group, its chalcogen analogues, and the –NC group have been added to the list of characteristic groups that are always cited as prefixes in substitutive nomenclature. Thus, when attached to a parent hydride these groups are named substitutively using the prefixes 'isocyanato', 'isothiocyanato', 'isoselenocyanato', 'isotellurocyanato', and 'isocyano', respectively, in preferred IUPAC names. In previous recommendations they were also expressed by functional class nomenclature.

(q) The potentially ambiguous names 'fulminate' and 'fulminato' are discarded in favor of systematic names.

8. Locants

(a) Superscript arabic numbers are now used to differentiate the nitrogen atoms of symmetrical geminal diamines, diimines, diamides, diimidamides, diamidines, dihydrazonamides and/or imidohydrazides, diamidrazones, and dihydrazonohydrazides and for nitrogen atoms that are not a part of the main chain in names of imidodi-, polyimido-, and di- and polynuclear acid chains, including di- and polycarbonic acids. Primes (′), double primes (″), triple primes (‴), etc., were used in previous recommendations

(b) Superscript arabic numbers are now used to locate chalcogen atoms of di- and polynuclear oxoacids, including di- and polycarboic acids. Online arabic numbers were used in previous recommendations.

(c) Numerical locants are no longer used in IUPAC names for urea, thiourea, condensed ureas, semicarbazide, semicarbazone, and the cation uronium.

(d) The locants N and N' are used for the $-NH_2$ and $=NH$ group of amidines, respectively rather than the locants N^1 and N^2 which were used in the 1979 recommendations (ref. 1).

9. Acyclic systems

(a) In a homogeneous acyclic structure the length of the chain is now preferred to unsaturation for choosing the preferred parent acyclic chain and the preferred parent chain of a preferred prefix; this is the reverse of these criteria from those in previous recommendations.

(b) The nomenclature for an $a(ba)_x$ heteroacyclic chain does not apply when the 'b' element is nitrogen or carbon; this is a change from the 1993 Guide (ref.2) where the 'amine' characteristic group present in such a system was not recognized and carbon was not excluded as a 'b' element.

10. Hantzsch-Widman system

(a) The final 'e' in Hantzsch-Widman names is required in preferred IUPAC names; it is still optional in general nomenclature. In the 1979 Rules (ref. 1), the final 'e' of a Hantzsch-Widman name was omitted when there was no nitrogen in the ring; in the 1993 Guide (ref. 2) the final 'e' was optional.

(b) The element mercury is removed from the Hantzsch-Widman system.

(c) Adapting the elements of Groups 1-12 to the principles of the Hantzsch-Widman nomenclature system is a major change, even though organometallic compounds involving these elements are only preselected at this time.

11. Polycyclic ring systems

(a) The use of indicated hydrogen (see P-14.7.1) for bridged fused ring systems, spiro ring systems (see P-24.3.2), and ring assemblies (see P-28.2.3) is now implemented in the same way as for mancude monocyclic and polycyclic fused ring systems (see P-25.7.1.1). The operation is simple and uniformly applied. The skeletal graph is first drawn and heteroatoms are added. Then, the maximum number of noncumulative double bonds are inserted, and finally indicated hydrogen is cited, consistent with the structure of the ring system, for all positions that are saturated, i.e., where there are two ring bonds and sufficient 'exo' bonds to satisfy the bonding number of the atom.

(b) A fusion name can only be used for preferred IUPAC names when at least two rings of five or more members are present, which is consistent with recommendations in the 1979 edition (ref. 1), but is a change from the recommendations in the 1999 publication on fused ring nomenclature (see FR-0, ref. 4) and the 1993 Guide (ref. 2) where no restriction was placed on the size or number of rings that must be present in order to use the principles of fusion nomenclature. In general nomenclature there is no restriction on the size or number of rings in a fused ring system.

(c) There is no elision of a vowel from fusion prefix names when followed by another vowel in preferred IUPAC names for fused ring systems as prescribed by P-25.3.1.3, which follows Rule R-2.4.1.1 of the 1993 Guide (ref. 2), which abrogated the elision recommended by Rule A-21.4 in the 1979 edition (ref. 1)

(d) Systematic 'benzo' names, for example 2*H*-1-benzopyran, are preferred IUPAC names for chromene, isochromene, chromane, isochromane, and their chalcogen analogues used in previous editions (refs. 1, 2, and 4)

(e) A new numbering system is now recommended for ring assemblies consisting of more than two rings or ring systems. The new locant system, composed of composite locants formed from a normal arabic number identifying each ring in order and a superscript number to represent the actual locants of the ring system itself, is recommended for preferred IUPAC names. The method used in earlier recommendations (refs. 1 and 2), involving serially primed actual locants may be used in general nomenclature.

(f) Unsaturation in ring assemblies is described by 'ene', 'yne', etc., endings cited after the closing brackets of the ring assembly name; this method allows ring assemblies with unsymmetrically located double bonds to be included in the method. This is a change from the 1979 and the 1993 Guide editions (refs. 1 and 2) and is completely consistent with the method established for spiro compounds in the 1999 publication on nomenclature of spiro compounds (ref. 8)

(g) The 'a' prefixes of replacement nomenclature for heterocyclic bridged fused, heterocyclic spiro ring systems, and heterocyclic ring assemblies are cited as nondetachable prefixes and are cited in front of the parent name. This technique allows naming of unsymmetrical heterocycles. Previously, replacement ('a') prefixes were cited with the name of the ring to which they belonged.

(h) The following names are now recommended as preselected (see P-12.2) bridge prefixes: 'sulfano' for –S–; 'disulfano' for –SS–; 'selano' for –Se–; 'tellano' for –Te–; 'azano' for –NH–; epitriazano for –NH-NH-NH–; and –NH-N=N– for epitriaz[1]eno. The bridge prefixes 'epithio', 'epidithio', 'episeleno', 'epitelluro', and 'epimino' [ref. 4, FR-8.3.1(d)] may be used in general nomenclature.

12. Seniority

(a) Seniority of polycyclic ring systems is now facilitated by a hierarchical order of ring systems, including cyclic and acyclic phane systems. The seniority order of a polycyclic ring system between parent hydrides having the same number of identical heteroatoms, the same number of rings, and the same number of skeletal atoms listed in descending order of seniority as follows: spiro compounds > cyclic phane systems > fusion ring systems > bridged fused ring systems > von Baeyer systems > linear phane systems > ring assemblies. This ordering is a change from earlier recommendations.

(b) In accordance with the seniority of classes (see P-41), compounds such as R-NH-Cl, R-NH-NO, and $R\text{-}NH\text{-}NO_2$ are now named as derivatives of amides (see P-67.1.2.6) and compounds such as R-NH-OH are named as *N*-derivatives of the senior amine and not as *N*-derivatives of hydroxylamine, $NH_2\text{-}OH$ (see P-62.4, P-68.3.1.1) as in previous recommendations.

13. Adducts

Adducts composed solely of organic compounds have their individual components cited in formulas in the order of seniority of classes (see P-41) no longer according to the number of species in the adduct, nor in accordance with the alphanumerical order as recommended in the 1979 Recommendations (see Rule D-1.55, ref. 1) and in the revised Nomenclature of Inorganic Chemistry, 2005 Recommendations (ref. 12). For adducts composed of organic and inorganic compounds, organic compounds precede inorganic compounds in formulas. Names are formed by citing the names of individual components in the order of the formula. The use of order of seniority of classes, a universal system, as a ranking criterion has been preferred to the language dependent alphanumerical order for preferred IUPAC names and in general nomenclature.

14. Enclosing marks

(a) Names such as cyclohexanecarbonyl and benzenesulfonyl are enclosed in parentheses, even though they are simple prefixes, in order to facilitate name interpretation by avoiding the illusion that two parent hydrides are present. This is a change from the 1993 Guide (ref. 2)

(b) When following the normal nesting order for enclosing marks, two or more enclosing marks of the same level are consecutive because independent enclosing marks accommodating other factors such as stereodescriptors must be inserted into an independent nomenclature fragment. The enclosing mark for the independent nomenclature fragment is jumped to the next level to avoid confusion.

(c) In fused ring names, enclosing parentheses are used following the numerical prefixes 'bis', 'tris', etc. which indicate multiple occurrences of a parent component. This is a change from the recommendations in the 1998 publication on fusion (ref. 4).

(d) All locants which form part of the name of all heterocyclic components in spiro ring systems and phane systems are placed in brackets as in fused ring systems. In the previous recommendations (ref. 5 and ref. 8) the locants of the first cited component were not enclosed in brackets.

15. Esters

The multiplicative operation is applied to naming organic esters. In doing so, the bi- or polyvalent functional class name is the multiplier and as such must be cited as the last organyl group (alkanediyl, arylene, etc.) as a separate word immediately before the name of the acid component denoted by the anion name derived from the appropriate acid (see P-72.2.2.2) rather than alphabetically along with other monovalent organyl groups, as was done in earlier recommendations.

16. Amides

When an amide is the principal function, it must be named as such. Hence, an *N*-acyl group attached to a nitrogen atom of a heterocyclic system is now named as a pseudoketone (see P-64.3). The method of considering amides as substituents on heterocyclic ring systems, described in the 1993 Recommendations (ref. 2), is retained but only for general nomenclature (see also P-66.1.3).

17. Inorganic parent structures

(a) For consistency in the names of polynuclear oxoacids, the numerical infix 'di' has been uniformly used in naming dinuclear 'hypo' acids, for example, hypodiphosphorous acid, rather than hypophosphorous acid.

(b) Amides and hydrazides of nitric and nitrous acids are now named systematically based on nitric or nitrous amide and/or hydrazide, in accordance with the seniority order of classes rather than as nitro and nitroso amines; the latter names can be used in general nomenclature.

(c) Since the name 'disulfurous acid' is used for HO-SO-SO$_2$-OH in the *Nomenclature of Inorganic Chemistry* (ref. 12), it cannot be used in the systematic way for HO-SO-O-SO-OH. Accordingly, the preselected name for the latter is '1,3-dihydroxy-1λ^4,3λ^4-dithioxane-1,3-dione'; and the preselected name for the former is sulfuric sulfurous anhydride.

18. Radicals and ions

(a) Radicals derived from amines and amides are named using suffixes such as '-aminylidene', '-amidylidene', and 'carboxamidylidene'. In previous recommendations such radicals were named as derivatives of 'nitrene', 'aminylene', or 'λ^1-azane'.

(b) For choosing the senior parent radical, the senior parent anion, and the senior parent cation, the pertinent criterion is the maximum number of radical, anionic, or cationic centers at the skeletal atom first cited in the seniority order of classes (P-41): N > P > As > Sb > Bi > Si > Ge > Sn > Pb > B > Al > Ga > In > Tl > O > S > Se > Te > C. In previous recommendations the order was that for the skeletal replacement ('a') prefixes.

(c) The preferred IUPAC name of an anion formed by the removal of a hydron from the chalcogen atom (O, S, Se, and Te) of a peroxyacid characteristic group is formed by replacing the 'ic acid' or 'ous acid' ending of the acid name by 'ate' or 'ite', respectively. In previous recommendations (RC-83.1.6, ref. 3), such anions were named on the basis of an anionic parent hydride.

(d) The use of compound suffixes 'aminide', 'iminide' and 'aminediide' is a change from previous practice where parent anions H_2N^- and HN_2^{2-} were used to express amines and imines having negative charge(s).

(e) Zwitterionic compounds having the ionic centers in the same parent structure are not considered as neutral compounds to which suffixes can be added. In previous recommendations such zwitterionic compounds were considered neutral and suffixes could be added to them.

19. Isotopically modified compounds

(a) Isotopically modified atoms or groups that are not identically modified in equivalent positions are expressed separately. This is a change from Section H of the 1979 Recommendations (ref. 1) and Chapter R-8 of the 1993 Guide (ref. 2).

(b) Isotopically labeled hydrogen atoms in hydrogenated mancude ring systems that are not identically modified are expressed separately. This is a change from previous recommendations.

GLOSSARY

Attached component. A ring or ring system that is fused to a parent component in fusion nomenclature; there are first-order attached components, for example 'benzo' in benzo[*g*]quinoline and 'furo' and 'pyrrolo' in furo[3,2-*h*]pyrrolo[3,4-*a*]carbazole; second-order attached components, for example 'cyclopenta' in cyclopenta[4,5]pyrrolo[2,3-*c*]pyridine and 'pyrano' in pyrano[3′,2′:4,5]cyclohepta[1,2-*d*]oxepine; and so on.

Additive operation. A procedure involving the formal assembly of a structure from its component parts without loss of any atoms or groups, for example calcium chloride, styrene oxide, 1,1′-biphenyl, pentyloxy, decahydronaphthalene, and pyridin-1-ium.

Amplificant. A ring or ring system replacing superatom(s) in the amplification operation of phane nomenclature.

Amplification. An operation in phane nomenclature restoring rings or ring systems from superatoms representing them in a phane skeleton name.

Amplification prefix. Names of the amplificants restored from the superatoms cited as nondetachable prefixes in a phane parent name, for example: benzena and pyridina.

Bridge. In von Baeyer alicyclic ring systems, an unbranched chain of atoms, an atom, or a valence bond connecting two bridgehead atoms; in bridged fused ring systems, a bridge can be an atom or a group of atoms, for example ethano, azano, and epoxireno.

Bridgehead atom. In von Baeyer alicyclic ring systems, any skeletal atom of the ring system that is bonded to three or more skeletal atoms (excluding hydrogen). In bridged fused ring systems, an atom of the fused system to which a bridge is attached.

Carbane nomenclature. Principles, rules, and conventions of substitutive nomenclature applied to the parent hydrides of carbon leading to names such as methanamine and cyclohexanol.

Characteristic group. A single heteroatom, such as –Cl, and =O; a heteroatom bearing one or more hydrogen atoms or other heteroatoms, such as $-NH_2$, –OH, $-SO_3H$, $-PO_3H_2$, and $-IO_2$; or a heteroatomic group attached to or containing a single carbon atom, for example –CHO, –CN, –COOH, and –NCO, attached to a parent hydride.

Complex substituent group. A substituent group consisting of a simple substituent group (the parent substituent group) to which is attached a compound substituent group, for example (chloromethyl)phenyl ($ClCH_2$-C_6H_4–).

Composite locant. A locant composed of two or more parts. In phane nomenclature composite locants are composed of a primary number identifying each amplificant and a superscript number expressing the locant of the amplificant itself, for example 1^1 and 1^2. In ring assemblies, composite locants consist of an arabic primary number, identifying each ring system, and an arabic superscript number expressing the numbering of the ring or ring system itself, for example 1^1 and 1^2.

Compound substituent group. A substituent group consisting of two parts, (1) a simple substituent group (the parent substituent group); and (2) one or more simple substitutive atoms or groups, for example, chloromethyl ($ClCH_2$–), hydroxysulfanyl (HO-S–), 2,2-dichloroethyl (Cl_2CH-CH_2–) .

Concatenated substituent group. A compound or complex substituent group formed only by the additive operation, for example sulfanyloxy (HS-O–) and cyclohexyloxy (C_6H_{11}-O–).

Detachable prefix. A substituent prefix cited before the name of a parent structure and, with the exception of hydro/dehydro prefixes, subject to alphabetization, for example amino, methyl, and silyl.

Functional class nomenclature. A system in which the principal characteristic group is expressed as a class term, such as chloride, alcohol, or ketone, written as a separate word or words, following a term derived from a parent hydride, for example methyl iodide and ethyl methyl ketone or substituent group, for example: acetyl chloride.

Functionalized parent hydride. A parent hydride with a characteristic group cited as a suffix, for example cyclopentanecarbonitrile.

Functional parent compound. A structure the name of which expresses or implies the presence of one or more characteristic groups and which has one or more substitutable hydrogen atoms attached to at least one of its skeletal atoms, or in which one of its characteristic groups can form at least one kind of functional modification, for example acetic acid, aniline, and phosphonic acid.

Functional replacement nomenclature. A method by which oxygen atoms of characteristic groups and functional parent compounds are replaced by halogen, chalcogen, and/or nitrogen atoms, for example propane-1-thiol and carbonimidic acid. It is a subset of replacement nomenclature, for which see below.

Fusion atom. An atom of a fused ring system which is common to two or more rings.

Fusion nomenclature. A system for naming bi- and polycyclic systems having two or more rings or ring systems joined together by two adjacent common atoms, for example, benzo[*g*]quinoline and cyclopenta[*a*]naphthalene.

General (IUPAC) nomenclature. The principles, rules, and conventions by which names other than preferred IUPAC names (PINs) are generated, for example acetone, propane-1,3-sultim, and thioacetamide.

Generalized 'ane' nomenclature. The principles, rules, and conventions of substitutive nomenclature generally applied to parent hydrides of elements in Groups 13, 14, 16 , and 17, for example sulfane, diazane, trisilane, and borane.

Hantzsch-Widman name. A name for a heteromonocyclic ring having three- through ten-ring members formed by the original proposals of Hantzsch and Widman in which a prefix or prefixes denoting the hetero atom(s) in the ring is added to stems denoting the size and degree of saturation of the ring, for example 1,2,4-triazole and 1,2-oxazole.

Heterane nomenclature. The principles, rules, and conventions of substitutive nomenclature applied to parent hydrides for elements of Groups 13, 14, 15, 16, and 17, other than carbon, for example disulfane, triarsane, disilane, and borane.

Heteroamine. A compound having an amino group bonded to a heteroatom, for example piperidin-1-amine.

Heteroimine. A compound having an imino group doubly bonded to a heteroatom, for example methylphosphanimine.

Heteroatom. An atom other than carbon belonging to Groups 13, 14, 15, 16, or 17 in the nomenclature of organic compounds, for example N, Si, and Ge.

Heterol. A compound having a hydroxy group bonded to a heteroatom, for example piperidin-1-ol.

Heterone. A compound having an oxygen atom doubly bonded to a heteroatom, for example methylsilanone.

Interior atom. An atom of a fused ring system that is not a peripheral atom.

Ketone. A compound having an oxygen atom doubly bonded to a carbon atom that is itself linked to two carbon atoms, for example propan-2-one (CH_3-CO-CH_3).

Multiplicative nomenclature. A system that allows the expression of two or more identical cyclic parent hydrides or heteroacyclic parent structures linked by di- or polyvalent substituent groups, for example 1,1′-peroxydibenzene and 4,4′- oxydi(cyclohexane-1-carboxylic acid).

Nondetachable prefix. A structure modifying prefix cited before the name of a parent structure and after alphabetized detachable prefixes and the detachable prefixes hydro and/or dehydro prefixes, for example bicyclo, spiro, aza, and nor.

Parent component. The parent component of a fused ring system is the ring or ring system having the highest seniority according to the seniority order of rings and ring systems, for example oxepine in dibenzo[*c*,*e*]oxepine.

Parent compound (often used in place of Parent structure; see Parent structure)

Parent hydride. An unbranched acyclic, a cyclic structure, or an acyclic/cyclic structure having a systematic or retained name and to which only hydrogen atoms are attached, for example methane, cyclohexane, styrene, and pyridine.

Parent structure. A parent hydride, for example methane; a functional parent compound, for example phenol; a functionalized parent hydride, for example propan-2-one.

Parent substituent group. A simple substituent group attached to a parent hydride or parent structure in a compound substituent group, for example the ethyl group in $ClCH_2$-CH_2–.

Peripheral atom. Any atom that forms part of the outer perimeter of a fused ring system.

Phane parent skeleton. The skeletal graph before the simplication operation and after the amplification operation in phane nomenclature.

Preferred IUPAC name (PIN). A name preferred among two or more names generated from two or more IUPAC recommendations including the many synonyms that have been coined and used over the years, for example disilylacetic acid and 3-chloropropanoic acid.

Preselected name. A name chosen for a noncarbon (inorganic) structure to be used as the basis for derivation of a preferred IUPAC name in the nomenclature of organic compounds, for example hydrazine and disulfane.

Primary locant. In phane nomenclature, an arabic number designating an atom or an amplificant in a phane parent skeleton. In ring assemblies, primary locants designate the rings or ring systems in the numbering of a structure.

Principal characteristic group. The characteristic group chosen for citation at the end of a name by means of a suffix or a class name, or implied by a trivial name, for example, ethanol and acetic acid.

Pseudoester. A compound having the generic formula $R\text{-}E(=O)_x(OZ)$ and chalcogen analogues where $x = 1$ or 2, and Z is not a carbon atom but an element from the following list: B, Al, In, Ga, Tl, Si, Ge, Sn, Pb, N(cyclic), P, As, Sb, Bi, for example silyl acetate.

Pseudoketone. A cyclic compound having a carbonyl group linked to one or two skeletal heteroatoms or an acyclic compound, other than esters or acid anhydrides, having a carbonyl group linked to one carbon atom and one skeletal heteroatom, except for nitrogen and halogens, or an acyclic compound having a carbonyl group linked to a heteroatom belonging to a ring or ring system, for example piperidin-2-one, 1-silylethan-1-one and 1-(piperidin-1-yl)ethan-1-one

Replacement nomenclature. A system in which one single nonhydrogen atom or a group of atoms is exchanged for another single nonhydrogen atom or group of atoms, for example 6λ^5-phosphaspiro[4.5]decane and phosphorothioic acid. Skeletal replacement, for which see below, and functional replacement nomenclature, for which see above, are subsets of replacement nomenclature.

Retained name. A traditional or common name used either as the preferred IUPAC name or as an alternative name in general nomenclature, for example acetone and aniline.

Semi-systematic name or semi-trivial name. A name in which only a part is used in a systematic sense, for example methane, but-2-ene, and chalcone.

Simple. A term for a single basic element, a simple substituent group consisting of just one part that describes an atom, or group of atoms as a unit, for example methyl ($–CH_3$), hydroxy (–OH), nitrilo (–N<), and propan-2-yl [$(CH_3)_2CH–$]. In bridged fused names, an atom or group of atoms described as a single unit is a simple bridge, for example epoxy, butano, and phospheno.

Simple substituent group. A substituent group with a name consisting of a single part that describes an atom or group of atoms as a unit, for example methyl ($–CH_3$), hydroxy (–OH), imino (=NH), and propan-2-yl [$(CH_3)_2CH–$].

Simplification. An operation in phane nomenclature leading to a simplified skeleton by condensing a ring or ring system to a single atom called a superatom.

Skeletal replacement (‘a’) nomenclature. A system in which a heteroatom replaces skeletal atoms of a homogeneous parent hydride, for example 8-thia-2,4,6-trisiladecane and 1,2-dicarba-*closo*-dodecaborane(12). It is a subset of replacement nomenclature for which see above.

Spiro nomenclature. A system for naming polycyclic systems with at least one spiro union based on nomenclature for monospiro bicyclic compounds developed by Adolf von Baeyer, for example spiro[4.5]decane.

Subsidiary parent substituent group. A parent substituent attached to the primary parent substituent group of a complex substituent group attached to a parent hydride or a parent structure, for example in the complex substituent group name (2- chloroethyl)phenyl, $Cl\mathbf{CH_2}\text{-}\mathbf{CH_2}\text{-}C_6H_4–$, the ethyl group is a subsidiary parent substituent group and the phenyl group the parent substituent group.

Substituent. An atom or group that takes the place of a substitutable hydrogen atom of a parent hydride or parent structure, for example amino, sulfanyl, and methyl.

Substitutive nomenclature. A system involving the exchange of one or more hydrogen atoms of a parent hydride or parent structure, except for hydrogen atoms of a chalcogen atom, by another atom or group of atoms expressed by a suffix or a prefix denoting the atom or group being introduced, for example 1-methylnaphthalene and pentan-1-ol.

Subtractive operation. A method for describing the removal of an atom, ion, or group implicit in a name. Prefixes, suffixes or endings are used, for example 3-norlabdane, propan-2-yl, and hex-2-ene.

Superatom. Atom in a simplified skeleton of a phane system resulting from the simplification of rings or ring systems.

Systematic name. A name composed entirely of specially coined or selected syllables with or without numerical prefixes and other structural symbols and constructed following the rules of a systematic nomenclature, for example cyclopropanecarbonitrile and 2-chloroethan-1-ol.

Trivial name. A name no part of which is used in a systematic sense, for example xanthophyll.

von Baeyer nomenclature. A system for naming polycyclic systems based on the system for naming bicyclic aliphatic ring systems developed by Adolf von Baeyer and including its extension to polycyclic ring systems, for example bicyclo[3.2.1]octane.

Chapter P-1 GENERAL PRINCIPLES, RULES, AND CONVENTIONS.

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P-11 Scope of nomenclature for organic compounds
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P-10 INTRODUCTION

For nomenclature purposes, a structure containing at least one carbon atom is considered to be an organic compound and can be named using the principles of organic nomenclature, such as substitutive or replacement nomenclature, as described in this book.

The formation of a systematic name for an organic compound requires first selection and then naming of a parent structure. This basic name may then be modified by prefixes, infixes, and, in the case of a parent hydride, suffixes, which convey precisely the structural changes required to generate the compound in question from the parent structure. In contrast to such systematic names, there are traditional names which are widely used both in industry and academic circles. Examples are acetic acid, benzene, and pyridine. Therefore, when they meet the requirements of utility and when they fit into the general pattern of systematic nomenclature, these traditional names are retained.

A major new principle is elaborated in these Recommendations; the concept of ‘preferred IUPAC names’ (PINs) is developed and systematically applied. Up to now, the nomenclature developed and recommended by IUPAC has emphasized the generation of unambiguous names in accord with the historical development of the subject. In 1993, due to the explosion in the circulation of information and the globalization of human activities, it was deemed necessary to have a common language that would prove important in legal situations, with manifestations in patents, export-import regulations, environmental and health and safety information, etc. However, rather than recommend only a single ‘unique name’ for each structure, we have developed rules for assigning ‘preferred IUPAC names’, while continuing to allow alternative names in order to preserve the diversity and adaptability of the nomenclature to daily activities in chemistry and in science in general.

Thus, the existence of preferred IUPAC names does not prevent the use of other names to take into account a specific context or to emphasize structural features common to a series of compounds. Preferred IUPAC names (PINs) belong to a ‘**preferred IUPAC nomenclature**’. Any name other than a preferred IUPAC name, as long as it is unambiguous and follows the principles of the IUPAC recommendations herein, is acceptable as a ‘general IUPAC name’, in the context of a ‘**general IUPAC nomenclature**’.

The concept of preferred IUPAC names is developed as a contribution to the continuing evolution of the IUPAC nomenclature of organic compounds. This book (Recommendations 2013) covers and extends the principles, rules, and conventions described in two former publications: *Nomenclature of Organic Chemistry*, 1979 Edition (ref. 1) and *A Guide to IUPAC Nomenclature of Organic Compounds, Recommendations 1993* (ref. 2). In a few instances, the 1979 rules and the 1993 recommendations have been modified to achieve consistency within the entire system. In case of divergence among various sets of recommendations, Recommendations 2013 prevail.

P-11 SCOPE OF NOMENCLATURE FOR ORGANIC COMPOUNDS

For nomenclature purposes we consider all compounds containing carbon as the principal element to be organic compounds as qualified above (see P-10). Oxygen, hydrogen, and nitrogen are the three elements usually associated with carbon to form the system of functional or characteristic groups. Other elements, among them the halogens and sulfur, complete the basic core of elements found in organic compounds. Substitutive nomenclature was first applied to compounds containing this set of atoms. The success of this type of nomenclature was such that it was extended to all elements of Groups 14, 15, 16, 17, and in Group 13, to boron; it could be extended to all elements of Group 13.

Table 1.1 Elements included in these recommendations

Groups	13	14	15	16	17
	B boron	C carbon	N nitrogen	O oxygen	F fluorine
	Al aluminium	Si silicon	P phosphorus	S sulfur	Cl chlorine
	Ga gallium	Ge germanium	As arsenic	Se selenium	Br bromine
	In indium	Sn tin	Sb antimony	Te tellurium	I iodine
	Tl thallium	Pb lead	Bi bismuth	Po polonium	At astatine

The elements Al, Ga, In, Tl have been added to the elements recommended in the 1979 edition (ref. 1) and the 1993 Guide (ref. 2)

The ending ‘ane’, characteristic of alkanes, was borrowed from methane, ethane, etc., and attached to terms forming the roots of the names of the various elements, for example sulfane, H_2S; phosphane, PH_3; silane, SiH_4; alumane, AlH_3. The resulting names constitute the basis of substitutive nomenclature; this treatment of parent hydrides is called **generalized ‘ane’ nomenclature** because all the rules applicable to alkanes are applicable to all hydrides of the elements of Groups 13, 14, 15, 16, and 17. The nomenclature of the carbon hydrides may be conveniently termed ‘**carbane nomenclature**’; whereas the term ‘**heterane nomenclature**’ covers the hydrides of elements other than carbon. Names of mononuclear parent hydrides are listed in Table 2.1 in Chapter P-2.

Organometallic compounds, i.e., compounds in which one or more carbon atom(s) is (are) directly attached to a metal atom, have been regarded as organic compounds for nomenclature purposes. This association is maintained in these recommendations (see P-69), for the metals, semimetals, and nonmetals included in Groups 13, 14, 15, 16, and 17. However, the nomenclature for other organic derivatives of the elements in Groups 1 through 12 is considered as part of the nomenclature of inorganic compounds.

Likewise, IUPAC preferred names for polymers and IUPAC preferred names for Natural Products and related compounds are outside the scope of this book. The former is to be developed in conjunction with the Polymer Committee on Polymer Terminology and the latter in conjunction with the IUPAC-IUBMB Joint Commission on Biochemical Nomenclature

The construction of systematic names is based on general nomenclature operations and rules, and on operations and rules specific to different types of nomenclature. These aspects are discussed in the following sections.

P-12 PREFERRED, PRESELECTED, AND RETAINED IUPAC NAMES

P-12.1 Preferred IUPAC names
P-12.2 Preselected names
P-12.3 Retained names
P-12.4 Methodology

P-12.1 PREFERRED IUPAC NAMES

Preferred IUPAC names are names for structures or structural components that are preferred among two or more names for the same structure generated from two or more recommended IUPAC rules for organic compounds or the many synonyms that have been coined and used over the years.

Preferred IUPAC names, or PINs for short, are names selected according to the set of principles, conventions, and rules given herein. They originate from the strict application of the rules; in this sense, they can be referred to as ‘single names’. All preferred IUPAC names for organic compounds are identified by the parenthetical abbreviation ‘(PIN)’ following the name. Names used in the past, but now discarded or no longer recommended, are placed in parentheses and preceded by the word ‘not’. Names of organic compounds based on aluminium, gallium, indium, and thallium are not followed by the parenthetical abbreviation (PIN), because the decision to choose between a name based on organic or inorganic principles has not yet been reached.

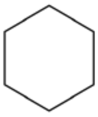
It is necessary to select a preferred alternative in many instances in the construction of the names of organic compounds. Preferred IUPAC names are given to parent structures; characteristic groups denoted by prefixes and suffixes used in PINs are designated as preferred prefixes or suffixes. They also result from the choice to be made among the different types of nomenclature, for example, substitutive nomenclature, functional class nomenclature, and multiplicative nomenclature; and among the different types of operations, for example substitutive, additive, and subtractive.

Most commonly, a **parent structure** is a **parent hydride**, i.e., a structure containing, in addition to one or more hydrogen atoms, a single atom of an element, for example, methane; or a number of atoms (alike or different) linked together to form an unbranched chain, for example, pentane; or a monocyclic or polycyclic ring system, for example, cyclohexane and quinoline. Methane is a retained name (see P-12.3) that is preferred to the systematic name 'carbane', a name never recommended to replace methane, but used to derive the names 'carbene' and 'carbyne' for the radicals $H_2C^{2\bullet}$ and $HC^{3\bullet}$, respectively. Similarly, the retained names 'ethane', 'propane', and 'butane' were never replaced by systematic names 'dicarbane', tricarbane', and 'tetracarbane' as recommended for analogues of silane, 'disilane'; phosphane, 'triphosphane'; and sulfane, 'tetrasulfane'. The name 'pentane' is formed by application of P-21.2.1 and is marked as the preferred IUPAC name, or PIN, even though no rule has been cited giving an alternative name. The same reasoning applies to cyclohexane, an IUPAC name resulting from the application of P-22.1.1. The name 'quinoline' is a retained name that is preferred to the alternative systematic fusion names '1-benzopyridine' or 'benzo[*b*]pyridine'.

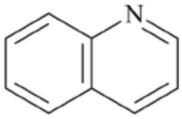
Examples:

CH_4
methane (preferred IUPAC name or PIN, a retained name)
carbane

CH_3-CH_2-CH_2-CH_2-CH_3
pentane (preferred IUPAC name or PIN)

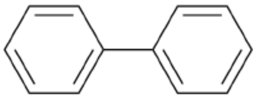


cyclohexane (PIN)

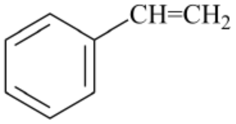


quinoline (PIN, a retained name, P-25.2.1)
1-benzopyridine (P-25.2.2.4)
benzo[*b*]pyridine (P-25.3.1.3)
(not 1-benzazine, see P-22.2.2.1.1)

It is sometimes convenient to employ parent hydrides of more complex structure, such as ring or ring-chain assemblies, for example biphenyl and styrene. The name '1,1′-biphenyl' results from the application of Rule P-28.2.1; it is the preferred IUPAC name and the locants '1,1″ are compulsory; the name 'biphenyl', without locants, can be used in general IUPAC nomenclature. The name 'styrene' is a retained name acceptable in general IUPAC nomenclature as being clear and unambiguous along with the substitutive name 'vinylbenzene'. The name 'ethenylbenzene' is the preferred IUPAC name (PIN).



1,1′-biphenyl (PIN)
biphenyl



styrene (a retained name; P-31.1.3.4)
vinylbenzene
ethenylbenzene (PIN; P-31.1.3.4)

A special class of parent structures having retained names (see P-12.3) is called **functional parent compounds**, for example, phenol and acetic acid. These two names are preferred IUPAC names; the corresponding systematic alternatives, benzenol and ethanoic acid, may be used in general IUPAC nomenclature. On the other hand, although acetone is a retained name recommended for general nomenclature, the preferred IUPAC name is the substitutive name propan-2-one.

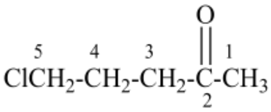
Examples:

C_6H_5-OH
phenol (PIN)
benzenol

CH_3-COOH
acetic acid (PIN)
ethanoic acid

CH_3-CO-CH_3
acetone
propan-2-one (PIN)

In order to generate the parent structure from a compound to be named, various formal **operations** must be carried out. For example, in naming the structure below, the parent hydride ‘pentane’ is formally derived by replacing the oxygen and chlorine atoms by the appropriate number of hydrogen atoms. When constructing the name, the formal operation is reversed; the suffix ‘one’ and the prefix ‘chloro’, indicating **substitution** of



$$\overset{5}{ClCH_2}\text{-}\overset{4}{CH_2}\text{-}\overset{3}{CH_2}\text{-}\underset{2}{\overset{O}{\overset{\|}{C}}}\text{-}\overset{1}{CH_3}$$

the hydrogen atoms of pentane, are attached to the name of the parent hydride to give the name ‘5-chloropentan-2-one’. Suffixes and prefixes can represent a number of different types of formal operations on the parent structure. Frequently, the suffix or prefix denotes the attachment of a characteristic group (functional group), for example, ‘one’ or ‘oxo’ for =O. A prefix may also describe a group derived from a parent hydride, for example ‘pentyl’, CH_3-CH_2-CH_2-CH_2-CH_2–, from pentane.

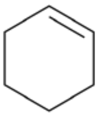
The **substitutive operation**, described in P-13.1, is the operation used most extensively in organic nomenclature. Indeed, the comprehensive nomenclature system based largely on the application of this operation to parent structures is, for convenience, termed **substitutive nomenclature**, although this nomenclature also involves many of the other types of operations described in P-13. Substitutive nomenclature is the set of **substitutive names, principles, conventions, and rules used for name construction.** Examples of substitutive and other nomenclature operations are shown in Table 1.2

Table 1.2 Nomenclature operations

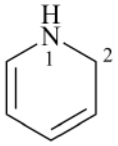
CH_3-CH_2-O-CH_2-CH_2-CH_3
1

CH_3-CHCl-CH_2-CO-CH_3
2

P(OCH_3)$_3$
3

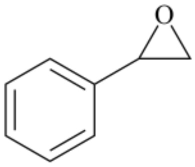


4



5

CH_3-O-CH_2-CH_2-O-CH_2-CH_2-O-CH_2-CH_2-O-CH_2-CH_3
6



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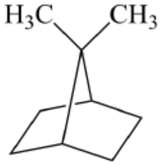

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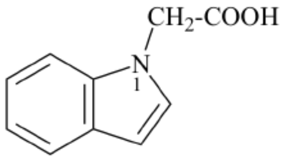

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Formula	Parent Structure (class name)	Operation	Name	Reference
1	propane (PIN) (ether)	substitutive functional class	1-ethoxypropane (PIN) ethyl propyl ether	P-13.1 P-13.3.3.2
2	pentane (PIN) (ketone)	substitutive functional class	4-chloropentan-2-one (PIN) 2-chloropropyl methyl ketone	P-13.1 P-13.3.3.2
3	phosphane (preselected name) (phosphite)	substitutive functional class	trimethoxyphosphane trimethyl phosphite (PIN)	P-13.1 P-13.3.3.2
4	cyclohexane (PIN)	substractive	cyclohexene (PIN)	P-31.1.3.1
5	pyridine (PIN)	additive	1,2-dihydropyridine (PIN)	P-31.2.3.1
6	ethane (PIN) tridecane (PIN)	substitutive skeletal (‘a’) replacement	1-ethoxy-2-[2-(2-methoxyethoxy)ethoxy]ethane 2,5,8,11-tetraoxatridecane (PIN)	P-13.1 P-13.2.1.1
7	oxirane (PIN) styrene + oxide	substitutive additive	phenyloxirane (PIN) styrene oxide	P-13.1 P-13.3.3.1
8	bornane bicyclo[2.2.1]heptane (PIN)	subtractive substitutive	10-norbornane 7,7-dimethylbicyclo[2.2.1]heptane (PIN)	P-13.4.3.2 P-13.1
9	acetic acid acetic acid + indole	substitutive conjunctive	(1*H*-indol-1-yl)acetic acid (PIN) 1*H*-indole-1-acetic acid	P-13.1 P-13.5.2

Another type of nomenclature expresses the principal characteristic group not as a suffix but as a term denoting its functional class cited in a name as a separate word; in Table 1.2, the name ‘ethyl propyl ether’ is a typical **functional class name** based on the functional class name ‘ether’. The corresponding substitutive name ‘1-ethoxypropane’ is constructed by using the prefix ‘ethoxy’ and the parent hydride name ‘propane’.

Substitutive and functional class names are written differently. Generally, substitutive names are unitary names that combine prefixes, names of parent hydrides, endings, and suffixes in one word. In contrast, a functional class name is written as separate words [in English], even though the part describing the parent hydride or the modified parent hydride is the result of the same operations used to construct substitutive names.

The great majority, if not all, of organic compounds can be named in accordance with the principles of substitutive and functional class operations. However, in these recommendations, where there is a choice, names obtained by the substitutive operation are preferred IUPAC names. In Table 1.2, examples 1, 2, and 3 illustrate this preference. The substitutive names 1-ethoxypropane and 4-chloropentan-2-one are preferred to the functional class names based on the names of the corresponding class, ether and ketone, ethyl propyl ether and 2-chloropropyl methyl ketone, respectively. In contrast, a functional class name is preferred for the ester 'trimethyl phosphite' to the substitutive name trimethoxyphosphane. Esters, along with acid halides, anhydrides, and amine oxides, linked to a nitrogen atom are preferably named by using functional class nomenclature; substitutive nomenclature is less preferred for naming these compound classes.

Other types of operations are widely used, alone or along with substitutive nomenclature. There are two major types of replacement operations, the skeletal replacement operation (often referred to as skeletal replacement nomenclature or simply 'a' nomenclature) and functional replacement nomenclature. The former is used as a necessary complement in order to introduce heteroatoms into cyclic hydrocarbons and to avoid highly complex prefixes in names for acyclic systems. For example, the name '2,5,8,11-tetraoxatridecane' formed by skeletal replacement is preferred to the substitutive name '1-ethoxy-2-[2-(2-methoxyethoxy)ethoxy]ethane' (see Table 1.2, example 6). The latter is used to derive a very large number of suffixes and prefixes from basic oxygen names. Additive and subtractive operations have been extended for naming radicals and ions. They are the sole method for modification of the degree of hydrogenation, by adding or subtracting pairs of hydrogen atoms. Examples 4 and 5 illustrate this methodology. The conjunctive operation eliminates hydrogen atoms from two different parent structures and then combines them; this method is used to name parent hydrides composed of repeated identical units or to link rings and chains under specific conditions. Example 9 in Table 1.2 illustrates such an operation; in IUPAC nomenclature, however, a substitutive name is always preferred to a conjunctive name, for example '(1*H*-indol-1-yl)acetic acid' is preferred to '1*H*-indole-1-acetic acid' (see P-51.1.2).

A nomenclature embraces the major operations along with the principles, conventions, and rules necessary to construct names of a particular type. Substitutive nomenclature and functional class nomenclature have been discussed above. Replacement nomenclature and conjunctive nomenclature also require specific principles, conventions, and rules. In contrast, additive and subtractive operations do not correspond to nomenclatures in their own right, but are necessary complements to other nomenclatures.

It is very important to recognize that, in general, the rules of the nomenclature of organic compounds are written in terms of classical valence bonding. The principles and general rules for the nomenclature of organic compounds are described in this Chapter. Substitutive nomenclature is then elaborated in Chapter P-2 (parent hydride names), in Chapter P-3 (endings, suffixes, and prefixes), and in Chapter P-4 (selection rules for parent structures and unique names). Chapter P-5 describes selection rules for construction of preferred IUPAC names. In Chapter P-6 the naming of compounds arranged in classes and groups related to the Periodic Table (Groups 13-17) is described. In Chapter P-7, nomenclature for radicals, ions, and related species is discussed. Chapter P-8 describes isotopic modifications of organic compounds. Chapter P-9 deals with configuration and conformation specification and Chapter P-10 deals with natural products. Preferred IUPAC names (PINs) for the natural products in Chapter P-10 are not identified. Although most of the names are in fact generally accepted, there is a nebulous grey area where a distinction between a natural product name and a systematic name based solely on principles of organic nomenclature has not been defined. This likely will be the task of a future project consisting of organic and biochemical nomenclaturists.

Several topics discussed in these recommendations have been published since 1993 as fully comprehensive documents: radicals and ions (ref. 3), fused and bridged fused ring systems (ref. 4), phane nomenclature (refs. 5, 6), the von Baeyer system for polycyclic compounds (ref. 7), spiro compounds (ref. 8), natural products (ref. 9), and fullerenes (refs. 10, 11). They are not reproduced *in extenso* in these recommendations. Rather, the principles, conventions, and rules are discussed in a less extensive manner. Readers should use the full publications to deal with more complex cases; these publications are not superseded in these recommendations unless specifically noted in boxed comments. Again, all modifications to previously published recommendations made to achieve consistency are clearly signalled in these recommendations and prevail over any former rules or interpretations.

In this book, the label 'PIN' is added to the names of compounds whose parent hydride contains at least one of the following elements: B, Si, Ge, Sn, Pb, N, P, As, Sb, Bi, O, S, Se, Te, Po, F, Cl, Br, I, At, and that also contain at least one carbon atom in their structure and that can be named by substitutive nomenclature or one of its related nomenclatures according to the principles described in these recommendations. (see P-11)

Rules for the selection of preferred IUPAC names (PINs) for compounds containing Al, Ga, In, Tl, as well as for compounds containing B, Si, Ge, Sn, Pb, N, P, As, Sb, Bi, O, S, Se, Te, Po, F, Cl, Br, I, At, and that do not contain carbon, or that cannot be named on the basis of the principles of organic nomenclature as described in this book will be discussed in a further publication. Examples are discussed in these recommendations to illustrate the scope and limitations of the substitutive nomenclature extended from carbon to all elements of Groups 13 through 17; the label 'preselected name' is added to appropriate names.

P-12.2 PRESELECTED NAMES

Preselected names are names for structures or structural components chosen among two or more names for noncarbon-containing (inorganic) parents to be used as the basis for preferred IUPAC names for organic derivatives in the nomenclature of organic compounds. Although systematic names alumane, gallane, indigane and thallane are preselected names, the names based on these parent hydrides currently do not have PIN status. However such names can be used in general nomenclature.

In the context of substitutive organic nomenclature, we need to select names for parent hydrides or other parent structures that do not contain carbon, in order to name derivatives that do contain carbon. The names chosen here for this purpose are termed 'preselected'. Each noncarbon-containing parent structure capable of substitution or functionalization by carbon-containing groups is assigned a unique 'preselected name’ to be used as the basis for deriving a preferred IUPAC name; noncarbon-containing characteristic groups, prefixes, and suffixes used in PINs are designated as preselected prefixes or suffixes.

Names of parent structures, prefixes, and suffixes identified herein as 'preselected' may not necessarily emerge as preferred IUPAC names in the context of inorganic chemical nomenclature.

All names listed in Table 2.1, with the exception of methane (carbane), are preselected names, and the concept is illustrated by the following examples.

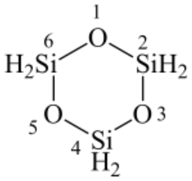
Examples:

SnH_3-$[SnH_2]_{11}$-SnH_3
tridecastannane (preselected name)

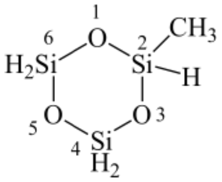
CH_3-SnH_2-$[SnH_2]_{11}$-SnH_3
1-methyltridecastannane (PIN)

$(HO)_3PO$
phosphoric acid (preselected name)

$(CH_3\text{-}O)_3PO$
trimethyl phosphate (PIN)



1,3,5,2,4,6-trioxatrisilinane (preselected name see P-22.2.2.1.6)
cyclotrisiloxane (P-22.2.6)



2-methyl-1,3,5,2,4,6-trioxatrisilinane (PIN)

P-12.3 RETAINED NAMES

Retained names are traditional or common, well-established names that may be either preferred IUPAC names, such as naphthalene, pyridine, and acetic acid; or preselected names, such as hydrazine and hydroxylamine; or as alternative names allowed in general nomenclature, for example, allene.

P-12.4 METHODOLOGY

In this book, names of parent structures, characteristic groups and their prefixes, and organic compounds are systematically identified as preferred IUPAC names, prefixes, and suffixes; or as preselected names, prefixes, or suffixes. Preferred IUPAC stereodescriptors are described and used in Chapter P-9. To facilitate the construction of the names of organic compounds, preferred and preselected prefixes for use in generating preferred IUPAC names are listed in Appendix 2 along with other prefixes that are acceptable in general nomenclature.

P-13 OPERATIONS IN NOMENCLATURE OF ORGANIC COMPOUNDS

The operations described in this section all involve structural modifications, and are classified first according to the type of modification, for example ‘replacement’; and then according to the way in which the modification is expressed, for example ‘by use of replacement infixes’. The structures to which the various modifications are applied can be regarded as parent structures, and the modifications are expressed by suffixes, affixes, infixes, and prefixes, or by a change of endings.

P-13.1 The substitutive operation
P-13.2 The replacement operation
P-13.3 The additive operation
P-13.4 The subtractive operation
P-13.5 The conjunctive operation
P-13.6 The multiplicative operation
P-13.7 The fusion operation
P-13.8 Operations used only in the nomenclature of natural products

P-13.1 THE SUBSTITUTIVE OPERATION

The substitutive operation involves the exchange of one or more hydrogen atoms for another atom or group of atoms. This process is expressed by a suffix or a prefix denoting the atom or group being introduced.

Examples:

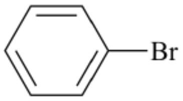
CH_3-CH_3
ethane (PIN)

$\longrightarrow$

CH_3-CH_2-SH
ethanethiol (PIN)
(substitutive suffix = ‘thiol’)

benzene (PIN)

$\longrightarrow$



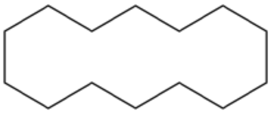
bromobenzene (PIN)
(substitutive prefix = ‘bromo’)

P-13.2 THE REPLACEMENT OPERATION

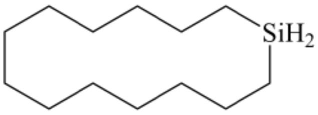
P-13.2.1 The replacement operation involves the exchange of one group of atoms or a single nonhydrogen atom for another. This can be expressed in several ways, as shown in the following subsections.

P-13.2.1.1 By replacement (‘a’) prefixes representing the element being introduced. This type of replacement is called ‘skeletal replacement’. The most common type of replacement in the nomenclature of organic compounds is replacement of carbon atoms by one or more of the following elements: O, S, Se, Te, N, P, As, Sb, Bi, Si, Ge, Sn, Pb.

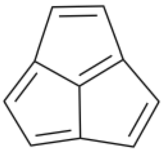
Examples:



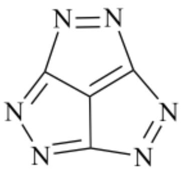
cyclotetradecane (PIN)



silacyclotetradecane (PIN)
[replacement (‘a’) prefix = ‘sila’]



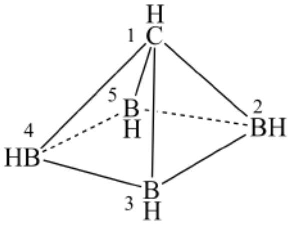
cyclopenta[*cd*]pentalene (PIN)



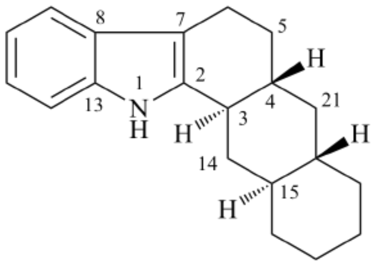
1,2,3,4,5,6-hexaazacyclopenta[*cd*]pentalene (PIN)
[replacement (‘a’) prefix = ‘aza’]

P-13.2.1.2 In specific instances, a heteroatom may be replaced by a carbon atom or by another heteroatom. The former is illustrated in the nomenclature of cyclic polyboranes (see IR-6.2.4.4, ref. 12) and both are found in natural products (see RF-5, ref. 9 and P-101.4) and must be applied only when specifically prescribed because the nomenclature of organic compounds is normally based on carbon atoms.

Examples:



1-carba-*nido*-pentaborane(5) (PIN)
[replacement ('a') prefix = 'carba'; carbon replacing boron; see P-68.1.1.2.1]



(4β*H*)-4-carbayohimban
[replacement ('a') prefix = 'carba'; carbon replacing nitrogen; see P-101.4]

P-13.2.2 By prefixes or infixes signifying replacement of oxygen atoms or oxygen-containing groups.

P-13.2.2.1 This type of replacement is called 'functional replacement'. The affixes represent the group(s) being introduced. Functional replacement nomenclature is described in P-15.5.

Examples:

$(CH_3)_2P(O){-}OCH_3$
methyl dimethylphosphinate (PIN)

→

$(CH_3)_2P(=NH){-}OCH_3$
methyl *P*,*P*-dimethylphosphinimidate (PIN)
[replacement infix = imid(o); =NH replaces =O]
methyl *P*,*P*-dimethyl(imidophosphinate)
(replacement prefix = 'imido'; =NH replaces =O)

$C_6H_5{-}P(O)(OH)_2$
phenylphosphonic acid (PIN)

→

$C_6H_5{-}P(\equiv N){-}OH$
phenylphosphononitridic acid (PIN)
[replacement infix = 'nitrid(o)'; ≡N replaces both =O and –OH]
phenyl(nitridophosphonic acid)
(replacement prefix = 'nitrido'; ≡N replaces both =O and –OH)

P-13.2.2.2 The affixes 'thio', 'seleno', and 'telluro' indicate replacement of an oxygen atom of a characteristic group by another chalcogen atom.

Examples:

$C_6H_5{-}COOH$
benzoic acid

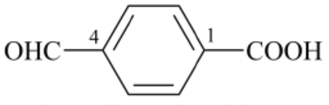
→

$C_6H_5{-}C\{O/Se\}H$
benzenecarboselenoic acid (PIN)
(replacement infix = 'selen(o)';
selenium replaces either =O or –O–)
selenobenzoic acid
(replacement prefix = 'seleno';
selenium replaces either =O or –O–)

$CH_3{-}[CH_2]_4{-}COOH$
hexanoic acid (PIN)

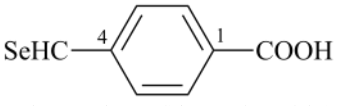
→

$CH_3{-}[CH_2]_4{-}C(S)SH$
hexane(dithioic) acid (PIN)
(replacement infix = 'thi(o)';
S replaces both =O and –O–)
(not hexanedithioic acid)



4-formylbenzoic acid (PIN)

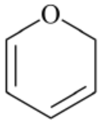
→



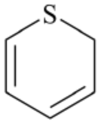
4-(methaneselenoyl)benzoic acid (PIN)
4-(selenoformyl)benzoic acid
(replacement prefix = 'seleno';
=Se replacing =O)

P-13.2.2.3 In specific instances, the prefixes ‘thio’, ‘seleno’, and ‘telluro’ indicate a skeletal modification. This replacement occurs with the cyclic parent hydrides having retained names, i.e., morpholine (see Table 2.3), pyran (see Table 2.2), chromene, isochromene, and xanthene (see Table 2.8), chromane and isochromane (see Table 3.1).

Example:



2*H*-pyran (PIN)
(not 2*H*-oxine, see P-22.2.2.1.1)



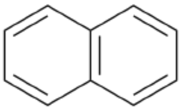
2*H*-thiopyran (PIN)
(replacement prefix = ‘thio’;
S replacing O)
2*H*-thiine (Hantzsch-Widman name)
(see P-22.2.2.1.1)

P-13.3 THE ADDITIVE OPERATION

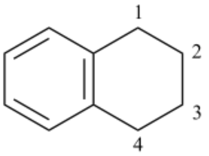
The additive operation involves the formal assembly of a structure from its component parts without loss of any atoms or groups. This operation can be expressed in several ways, as shown in the following subsections.

P-13.3.1 By an additive prefix

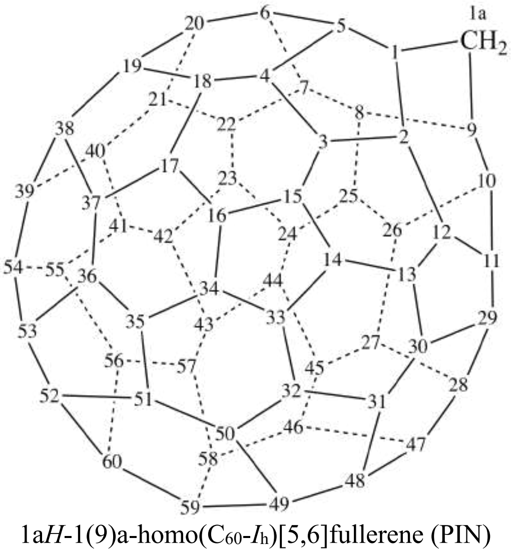
Examples:



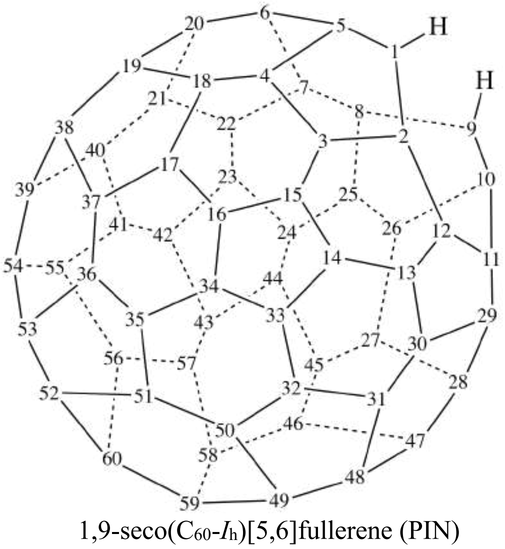
naphthalene (PIN)



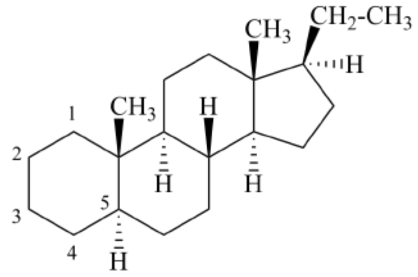
1,2,3,4-tetrahydronaphthalene (PIN)
(‘hydro’ = prefix designating addition
of one hydrogen atom)



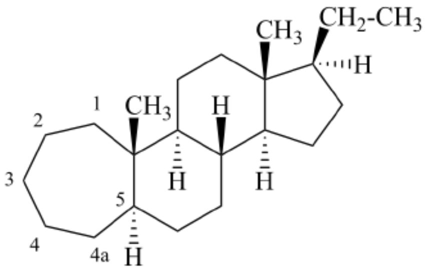
1a*H*-1(9)a-homo(C_{60}-I_h)[5,6]fullerene (PIN)



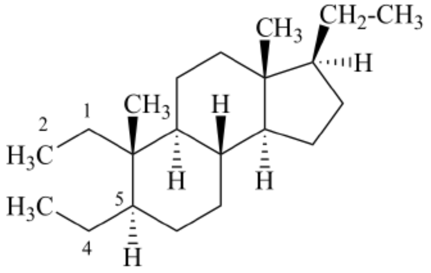
1,9-seco(C_{60}-I_h)[5,6]fullerene (PIN)



5α-pregnane



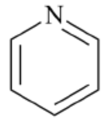
4a-homo-5α-pregnane
(‘homo’ = addition of a methylene group, –CH_2–, which in this case expands a ring, see P-101.3.2.1)



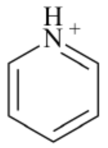
2,3-seco-5α-pregnane
(‘seco’ = addition of two hydrogen atoms at positions 2 and 3 made necessary by cleavage of the bond between C-2 and C-3)

P-13.3.2 By an additive suffix

Examples:



$+ H^+$ $\longrightarrow$



pyridine (PIN)

pyridin-1-ium (PIN)
(‘ium’ = suffix designating the addition of one H^+)

$CH_3\text{-}BH_2 + H^-$ $\longrightarrow$ $CH_3\text{-}BH_3^-$

methylborane (PIN)

methylboranuide (PIN)
(‘uide’ = suffix designating the addition of one H^-)

P-13.3.3 By a separate word

P-13.3.3.1 With the name of a neutral parent structure

Examples:

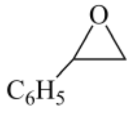
$CH_3\text{-}C{\equiv}N$ $\longrightarrow$ $CH_3\text{-}C{\equiv}NO$

acetonitrile (PIN)

acetonitrile oxide (PIN)

$C_6H_5\text{-}CH{=}CH_2$ $\longrightarrow$

styrene
ethenylbenzene (PIN)



styrene oxide
phenyloxirane (PIN)

P-13.3.3.2 With one or more substituent prefix name(s)

Here the separate word is a class or subclass name representing the characteristic group or the kind of characteristic group to which the substituents are linked (see also functional class nomenclature, P-15.2).

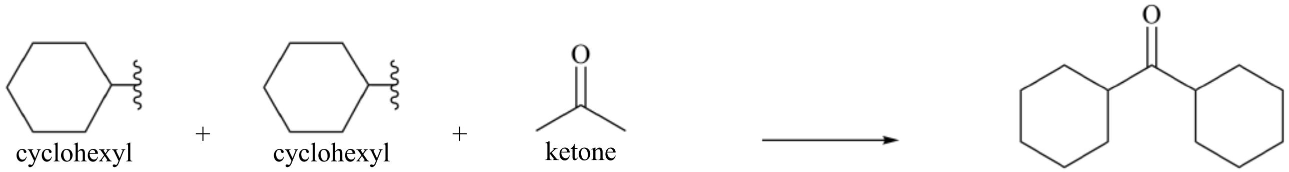
Examples:

CH_3– + –OH $\longrightarrow$ $CH_3\text{-}OH$

methyl (preferred prefix)

alcohol (class name)

methyl alcohol
methanol (PIN)



cyclohexyl (preferred prefix)	+	cyclohexyl (preferred prefix)	+	ketone (class name)	→	dicyclohexyl ketone dicyclohexylmethanone (PIN)
CH_3- methyl (preferred prefix)	+	C_6H_5- phenyl (preferred prefix)	+	–O– oxy (preselected prefix)	→	$CH_3-O-C_6H_5$ methyl phenyl ether anisole (PIN) methoxybenzene
$C_6H_5-CH_2-$ benzyl (preferred prefix)	+	–CN cyanide (class name)			→	$C_6H_5-CH_2-CN$ benzyl cyanide phenylacetonitrile (PIN)

P-13.3.4 By adding substituent groups together, in an operation called 'concatenation'

Examples:

$CH_3-CH_2-CH_2-CH_2-CH_2-$ pentyl (preferred prefix)	+	–O– oxy (preselected prefix)			→	$CH_3-CH_2-CH_2-CH_2-CH_2O-$ pentyloxy (preferred prefix)
Cl– chloro (preselected prefix)	+	–CO– carbonyl (preferred prefix)			→	Cl-CO– chlorocarbonyl carbonochloridoyl (preferred prefix)
–NH– azanediyl (preselected prefix)	+	$-CH_2-CH_2-$ ethane-1,2-diyl (preferred prefix)	+	–NH– azanediyl (preselected prefix)	→	$-NH-CH_2-CH_2-NH-$ ethane-1,2-diylbis(azanediyl) (preferred prefix)

P-13.3.5 By adding molecular entities together

Chemical species AB in which two molecular entities A and B are combined directly with no loss of atoms from either A or B can be named as adducts (see P-14.8) by citing the names of A and B linked with an 'em' dash.

Example:

CO carbon monoxide (PIN)	+	CH_3-BH_2 methylborane (PIN)	→	$CO \bullet BH_2-CH_3$ carbon monoxide—methylborane (1/1) (PIN)

P-13.4 THE SUBTRACTIVE OPERATION

The subtractive operation involves the removal of an atom or group implicit in a name. This operation can occur with no other change, with introduction of unsaturation, or with formation of substituent groups, radicals, or ions. Several prefixes are used to indicate subtractive operations of many kinds in natural products. Subtraction can be expressed in several ways as shown in the following subsections.

P-13.4.1 By a suffix

Examples:

CH_4 methane (PIN)	–	$H^{\bullet}$ monohydrogen (preselected name)	→	$CH_3^{\bullet}$ methyl (PIN; a radical; the suffix 'yl' indicates loss of one hydrogen atom)
CH_3-CH_3 ethane (PIN)	–	H^+ hydron (preselected name)	→	$CH_3-CH_2^-$ ethanide (PIN; an anion; the suffix 'ide' indicates loss of a hydron)

$CH_3\text{-}CH_2\text{-}CH_2\text{-}CH_3$ butane (PIN)	– H^- hydride (preselected name)	⟶	$CH_3\text{-}CH_2\text{-}CH_2\text{-}CH_2^+$ butylium (PIN; the suffix ‘ylium’ indicates loss of a hydride ion)

P-13.4.2 By a change of ending

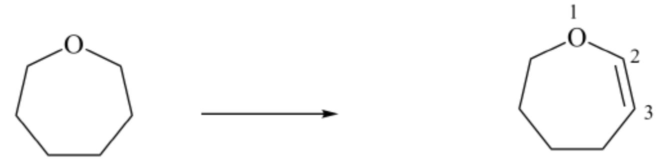
Examples:

$C_6H_5\text{-}SO_2\text{-}OH$ benzenesulfonic acid (PIN)	– H^+ hydron (preselected name)	⟶	$C_6H_5\text{-}SO_2\text{-}O^-$ benzenesulfonate (PIN; the ending ‘ate’ indicates loss of a hydron from an ‘ic acid’)
$CH_3\text{-}CH_2\text{-}CH_2\text{-}CH_3$ butane (PIN)	– 2 H hydrogen (preselected name)	⟶	$\overset{3}{C}H_3\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}H{=}CH_2$ but-1-ene (PIN; the ending ‘ene’ indicates loss of two hydrogen atoms)

P-13.4.3 By the prefixes ‘dehydro’ and ‘nor’

P-13.4.3.1 The prefix ‘dehydro’

Example:

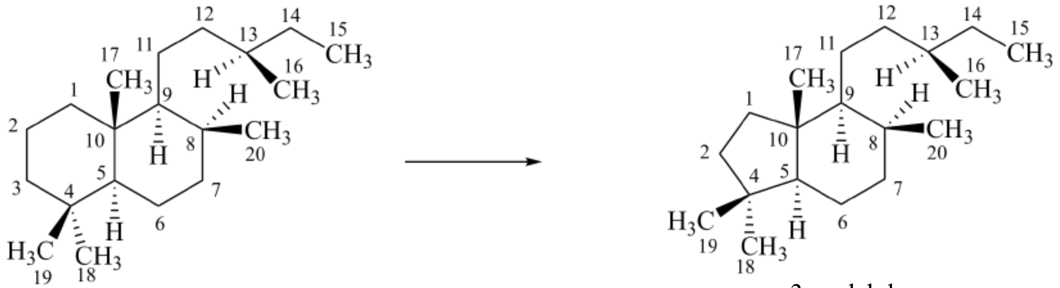


oxepane (PIN)

2,3-didehydrooxepane
(the prefix ‘didehydro’ indicates
loss of 2 hydrogen atoms)
2,3,4,5-tetrahydrooxepine
(PIN, see P-54.4.1)

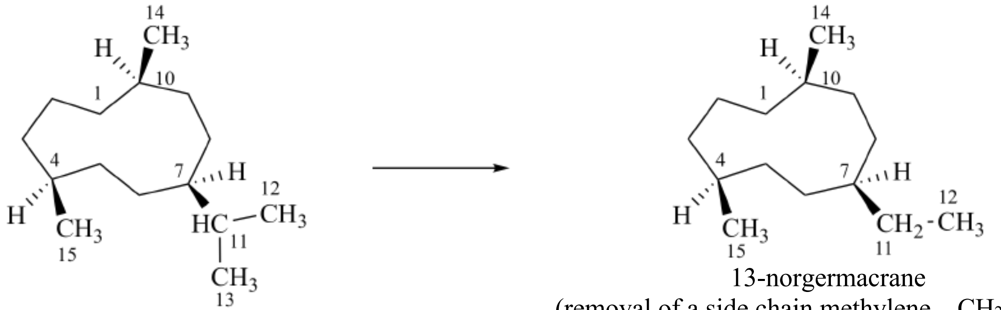
P-13.4.3.2 By the prefix ‘nor’

The prefix ‘nor’ is used to indicate removal of an unsubstituted saturated skeletal atom from a ring or a chain of a stereoparent structure with its attached hydrogen atom(s). It can also indicate the loss of a –CH= group from a mancude ring from a stereoparent structure (see P-101.3.1) and the loss of a carbon atom from a fullerene structure (see P-27.4.2). Examples:



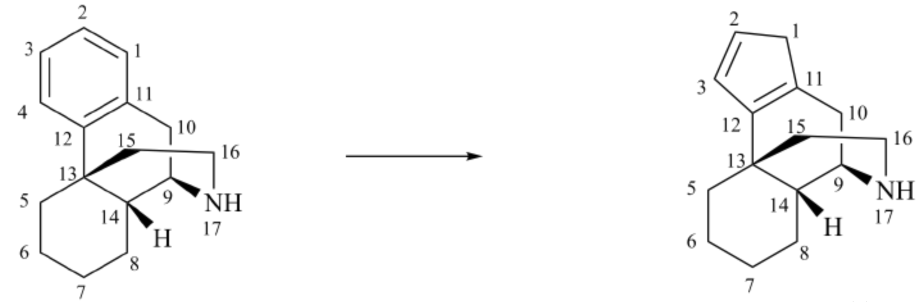
labdane
(fundamental parent structure)

3-norlabdane
(ring contraction by removal
of a ring methylene, $–CH_2–$, group)



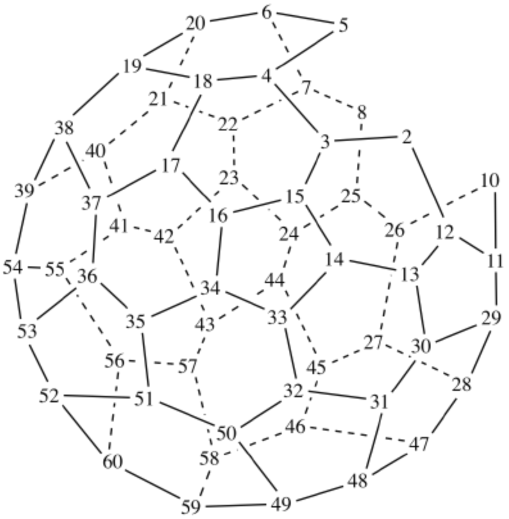
germacrane
(fundamental parent structure)

13-norgermacrane
(removal of a side chain methylene, $–CH_2–$, group)
(1*R*,4*s*,7*S*)-4-ethyl-1,7-dimethylcyclodecane
(see P-101.3.1.1)



morphinan
(fundamental parent structure)

1*H*-4-normorphinan



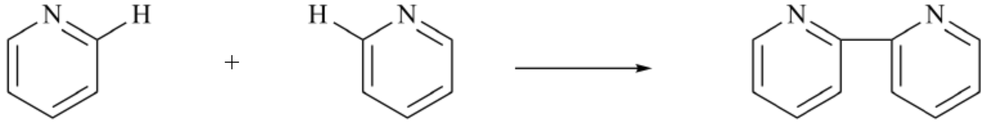
1,9-dinor(C_{60}-I_h)[5,6]fullerene (PIN)

P-13.5 THE CONJUNCTIVE OPERATION

The conjunctive operation involves the formal construction of a name for a compound from the names of its components with subtraction of the same number of hydrogen atoms from each component at each site of the junction. This operation is expressed as noted in the following subsections.

P-13.5.1 By placing a multiplicative prefix ‘bi’, ‘ter’, ‘quater’, etc. (see P-14.2.3) before the name of the corresponding parent hydride.

Example:



pyridine (PIN)

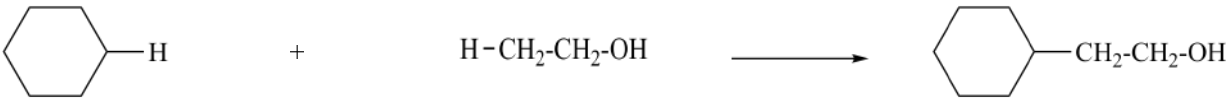
pyridine (PIN)

2,2′-bipyridine (PIN)
2,2′-bipyridyl (see P-28.2.1)

P-13.5.2 By juxtaposition of component names (conjunctive nomenclature)

This method is used by Chemical Abstracts Service. It is not recommended for constructing preferred IUPAC names; substitutive nomenclature is the recommended operation (see P-51). This method is most commonly used when the two components to be joined are a ring or a ring system and a carbon chain (or chains) substituted by the principal characteristic group of the compound. In this method, both the principal characteristic group and the ring, or ring system, must terminate the chain; the rest of the structure attached to the chain, if any, is described by substituent prefixes, the locations of which are indicated by Greek letter locants, α, α^1, β, β^1, etc. (α designates the atom next to the principal characteristic group).

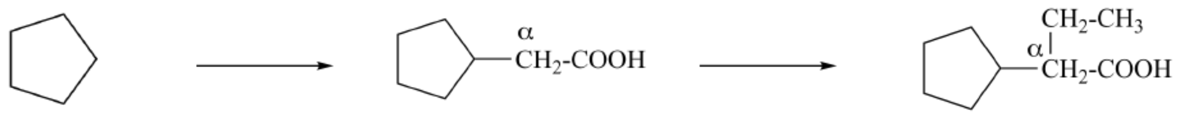
Examples:



cyclohexane (PIN)

ethanol (PIN)

cyclohexaneethanol
2-cyclohexylethan-1-ol (PIN)



cyclopentane (PIN)

cyclopentaneacetic acid
cyclopentylacetic acid (PIN)

α-ethylcyclpentaneacetic acid
2-cyclopentylbutanoic acid (PIN)

P-13.5.3 Ring formation

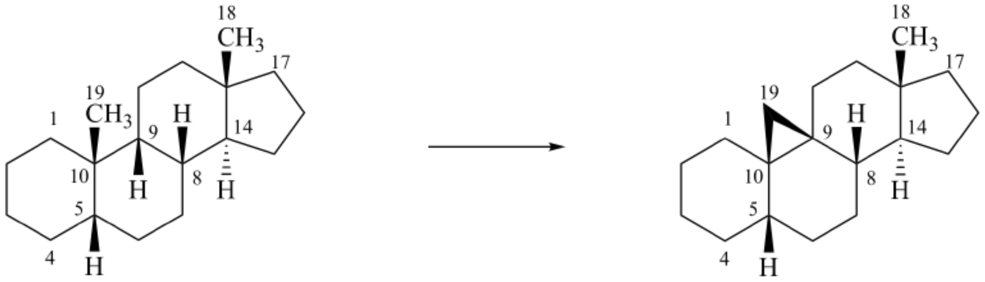
The formation of a ring by means of a direct link between any two atoms of a parent structure with loss of one hydrogen atom from each is indicated by the prefix ‘cyclo’.

Examples:

$CH_3\text{-}CH_2\text{-}CH_3$

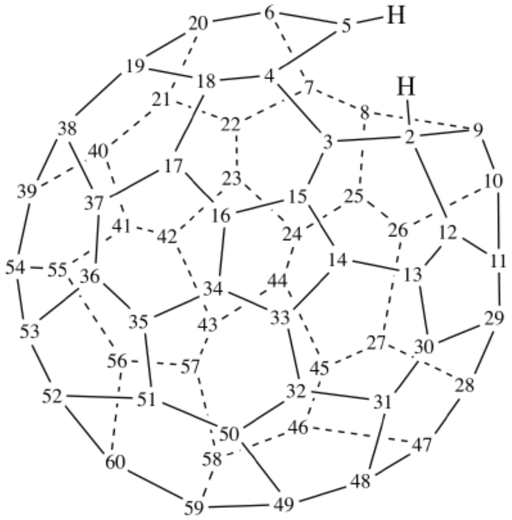
propane (PIN)

cyclopropane (PIN)



5β,9β-androstane
(fundamental parent structure)

9,19-cyclo-5β,9β-androstane
(see P-101.3.3)

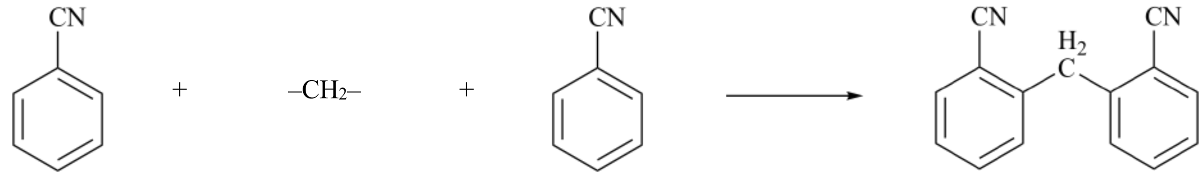


2*H*-2,9-cyclo-1-nor(C_{60}-*I*$_h$)[5,6]fullerene (PIN)

P-13.6 THE MULTIPLICATIVE OPERATION

This operation allows the expression of multiple occurrences of parent structures connected by a symmetrical multivalent structure.

P-13.6.1 In substitutive nomenclature the multiplicative operation is used to name assemblies of identical parent structures linked by di- or polyvalent substituent groups. Identical parent structures are functionalized parent hydrides, functional parents, and rings or ring systems. It is, in fact, substitutive nomenclature in which identical parent structures are interconnected by a di- or polyvalent substituent group.



benzonitrile (PIN)

methylene
(preferred prefix)

benzonitrile (PIN)

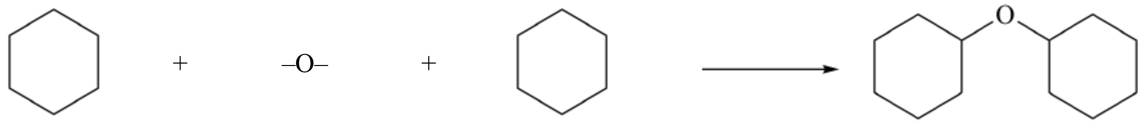
2,2′-methylenedibenzonitrile (PIN)

3 $CH_3\text{-}COOH$ + –N< ⟶ $N(CH_2\text{-}COOH)_3$

acetic acid

nitrilo
(preselected
prefix)

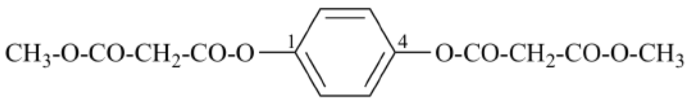
2,2′,2″-nitrilotriacetic acid
N,*N*-bis(carboxymethyl)glycine
(see P-103.1, Table 10.4)



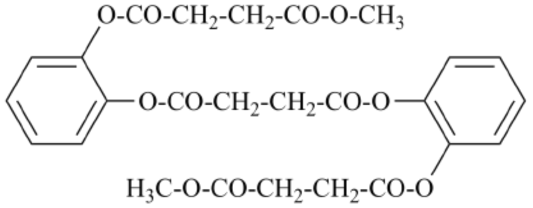
cyclohexane (PIN) | oxy (preferred prefix) | cyclohexane (PIN) | 1,1′-oxydicyclohexane (PIN)

P-13.6.2 In functional class nomenclature the multiplicative operation is used to name assemblies of identical parent structures linked by a bi- or multivalent functional class name.

Examples:



dimethyl 1,4-phenylene dipropanedioate (PIN)

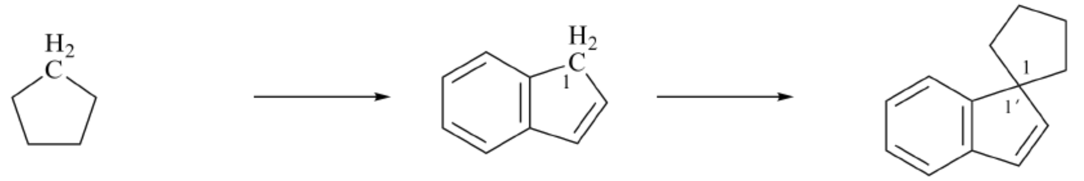


dimethyl butanedioylbis[oxy(2,1-phenylene)] dibutanedioate (PIN)

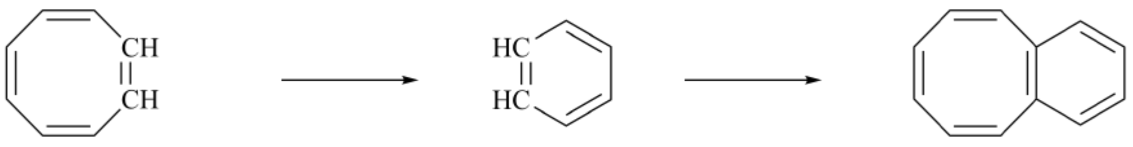
P-13.7 THE FUSION OPERATION

The fusion operation involves the union of two rings or ring systems so that atoms or atoms and bonds are common to each. Spiro systems have one atom in common; fused ring systems have both atoms and bonds in common.

Examples:



cyclopentane (PIN) | 1*H*-indene (PIN) | spiro[cyclopentane-1,1′-indene] (PIN)



8-annulene
cycloocta-1,3,5,7-tetraene (PIN)

benzene (PIN)

benzo[8]annuene
(PIN; see P-25.3.2.1.1)

P-13.8 OPERATIONS USED ONLY IN THE NOMENCLATURE OF NATURAL PRODUCTS

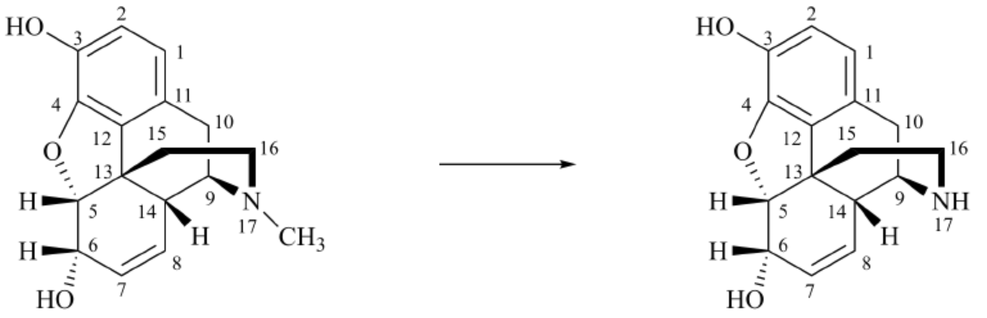
In the nomenclature of natural products several prefixes are used to indicate the loss of a group, i.e., the exchange of a group for hydrogen. The subtraction of the elements of water with concomitant bond formation can also be regarded as a subtractive operation. These operations are denoted by the following prefixes:

‘abeo’	rearrangement of single bonds in a stereoparent structure (see P-101.3.5.1)
‘anhydro’	loss of H_2O from two hydroxy groups with bond formation (see P-102.5.6.7)
‘apo’	removal of all of a side chain from a carotenoid system (see P-101.3.4.2)
‘de’	subtraction of an oxygen atom from an –OH group in carbohydrate nomenclature (see P-102.5.3) or exchange of a methyl group for a hydrogen atom (see P-101.7.5)
‘des’	removal of an amino acid residue from a peptide (see P-103.3.5.4) or of a terminal unsubstituted ring from a steroid skeleton (see P-101.3.6)
‘*retro*’	moving double bonds from a carotenoid system (see P-101.3.5.2)

P-13.8.1 By the prefixes ‘de’ and ‘des’

P-13.8.1.1 The prefix ‘de’ (not ‘des’), followed by the name of a group or atom (other than hydrogen), denotes removal (or loss) of that group and addition of the necessary hydrogen atoms, i.e., exchange of that group with hydrogen atoms.

Example:



HO
3
2
1
11
4
10
12
15
16
O
13
H
5
14
9
N
17
CH3
H
6
H
8
HO
7
HO
3
2
1
11
4
10
12
15
16
O
13
H
5
14
9
NH
17
H
6
H
8
HO
7

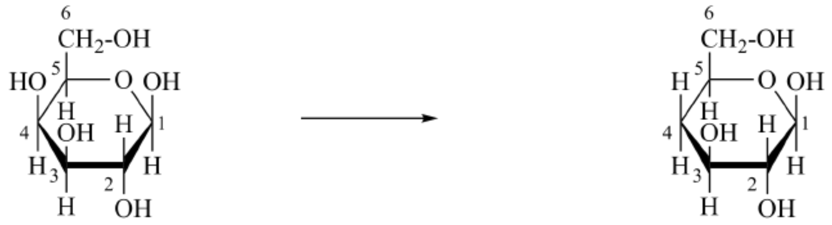
I morphine

II demethylmorphine
(exchange of methyl for H)

I (5βH)-17-methyl-7,8-didehydrofuro[2′,3′,4′,5′:4,12,13,5]morphinan-3,6α-diol
4,5α-epoxy-17-methyl-7,8-didehydromorphinan-3,6α-diol
II (5βH)-7,8-didehydrofuro[2′,,3′,,4′,,5′,:4,12,13,5]morphinan-3,6α-diol
4,5α-epoxy-7,8-didehydromorphinan-3,6α-diol

As an exception, ‘deoxy’, when applied to hydroxy compounds, denotes the removal of an oxygen atom from an –OH group with the reconnection of the hydrogen atom. ‘Deoxy’ is extensively used as a subtractive prefix in carbohydrate nomenclature (see P-102.5.3).

Example:



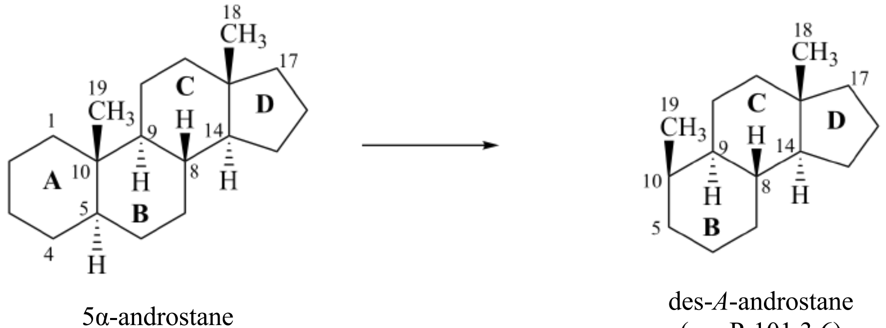
6
CH2-OH
HO
5
O
OH
H
4
OH
H
1
H
3
H
2
H
OH
6
CH2-OH
H
5
O
OH
H
4
OH
H
1
H
3
H
2
H
OH

β-D-galactopyranose
(fundamental parent structure)

4-deoxy-β-D-*xylo*-hexopyranose
(not 4-deoxy-β-D-*xylo*-galactopyranose)
(2*R*,3*R*,4*S*,6*S*)-6-(hydroxymethyl)oxane-2,3,4-triol
(numbering based on the parent hydride oxane)

P-13.8.1.2 The prefix ‘des’ signifies removal of an amino acid residue of a polypeptide, with rejoining of the chain (see P-103.3.5.4) or the removal of a terminal ring of a stereoparent (see P-101.3.6).
Examples:

oxytocin ⟶ des-7-proline-oxytocin
(removal of the proline residue at
position 7 of oxytocin)



18
CH3
17
19
CH3
C
H
D
1
9
14
A
10
H
8
H
5
B
4
H
18
CH3
17
19
CH3
C
H
D
9
14
10
H
8
H
5
B

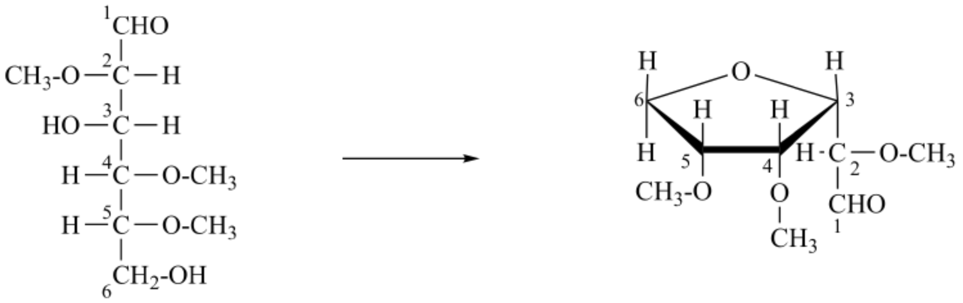
5α-androstane
fundamental parent structure)

des-*A*-androstane
(see P-101.3.6)
(removal of ring A of 5α-androstane)

P-13.8.2 By the prefix ‘anhydro’

Intramolecular ethers, formally arising by elimination of water from two hydroxy groups of a single molecule of a monosaccharide (aldose or ketose) or monosaccharide derivative, is indicated by the detachable prefix ‘anhydro’ preceded by a pair of locants identifying the two hydroxy groups involved. The prefix ‘anhydro’ is placed in a name in accordance with the principles of alphabetical order (see P-102.5.6.7.1).

Example:



2,4,5-tri-*O*-methyl-D-mannose
(fundamental parent structure)

3,6-anhydro-2,4,5-tri-*O*-methyl-D-mannose
(the prefix 'anhydro' describes removal of H_2O
from 2 'OH' groups in the same structure)

P-14 GENERAL RULES

P-14.0 Introduction
P-14.1 Bonding number
P-14.2 Multiplicative prefixes
P-14.3 Locants
P-14.4 Numbering
P-14.5 Alphanumerical order
P-14.6 Nonalphanumerical order
P-14.7 Indicated and 'added indicated hydrogen'
P-14.8 Adducts

P-14.0 INTRODUCTION

Rules described in this section are of general application for naming types of compounds and individual compounds. They must be closely followed to construct preferred IUPAC names as well as names for general use.

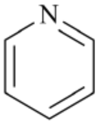
P-14.1 BONDING NUMBER

The concept of a standard valence state for an atom is fundamental to organic nomenclature. Since most organic names are derived by formal exchange of hydrogen atoms of a parent structure for other atoms or groups, it is necessary to know exactly how many hydrogen atoms are implied for skeletal atoms of the parent structure. For example, does the name phosphane refer to PH_3 or PH_5 ? This is a problem when an element can occur in more than one valence state; in such cases, the standard state is normally not specified, but any other valence state is noted by citation of an appropriate **bonding number**. More details are given in the publication 'Treatment of Variable Valence in Organic Nomenclature (Lambda Convention)' (ref. 13). In these Recommendations, this convention is called simply the 'λ-convention'.

P-14.1.1 Definition.

The bonding number '*n*' of a skeletal atom is the sum of the total number of bonding equivalents (valence bonds) of that skeletal atom to adjacent skeletal atoms, if any, in a parent hydride and the number of hydrogen atoms.

Examples:

H_2S	for S, $n = 2$
H_6S	for S, $n = 6$
$(C_6H_5)_3PH_2$	for P, $n = 5$
	for N, $n = 3$

P-14.1.2 Standard bonding numbers. The bonding number of a skeletal atom is standard when it has the value given in Table 1.3.

Table 1.3 Standard bonding numbers for the elements of Groups 13, 14, 15, 16, and 17

Standard bonding number (*n*)	**Element**				
3	B	Al	Ga	In	Tl
4	C	Si	Ge	Sn	Pb
3	N	P	As	Sb	Bi
2	O	S	Se	Te	Po
1	F	Cl	Br	I	At

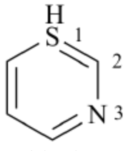
P-14.1.3 Nonstandard bonding numbers

A nonstandard bonding number of a **neutral** skeletal atom of a parent hydride is indicated by the symbol ‘λ^n’, cited in conjunction with an appropriate locant. Note that the ‘*n*’ in the symbol ‘λ^n’ is italicized but the numbers in a specific symbol, e.g., ‘λ^4’, are not (for the use of italicized ‘*n*’ in the symbol ‘λ^n’, see the General rules for symbols in physical quantities, Section 1.3 in ref. 14).

Examples:

$CH_3\text{-}SH_5$
methyl-λ^6-sulfane (PIN)

$(C_6H_5)_3PH_2$
triphenyl-λ^5-phosphane (PIN)



1λ^4,3-thiazine (PIN)

P-14.2 MULTIPLICATIVE PREFIXES

Three types of multiplicative prefixes are used in names to denote multiplicity of identical features in structures (characteristic groups, substituent groups, multiple bonds) and correspondingly of affixes (suffixes, infixes, and prefixes) in names. They are always placed before the part of the name to which they relate.

P-14.2.1 Basic multiplicative prefixes denote simple features and, in general, are the first choice among such prefixes to specify multiplicity (ref. 15). They are listed in Table 1.4.

Table 1.4 Basic numerical terms (multiplicative prefixes)

Number	Numerical Term	Number	Numerical Term	Number	Numerical Term	Number	Numerical Term
1	mono, hen	11	undeca	101	henhecta	1001	henkilla
2	di,do	20	icosa	200	dicta	2000	dilia
3	tri	30	triaconta	300	tricta	3000	trilia
4	tetra	40	tetraconta	400	tetracta	4000	tetralia
5	penta	50	pentaconta	500	pentacta	5000	pentalia
6	hexa	60	hexaconta	600	hexacta	6000	hexalia
7	hepta	70	heptaconta	700	heptacta	7000	heptalia
8	octa	80	octaconta	800	octacta	8000	octalia
9	nona	90	nonaconta	900	nonacta	9000	nonalia
10	deca	100	hecta	1000	kilia		

P-14.2.1.1 The prefix mono

P-14.2.1.1.1 When alone, the numerical term for the number ‘1’ is ‘mono’ and that for ‘2’ is ‘di’. In association with other numerical terms, the number ‘1’ is represented by ‘hen’ (except in the case of ‘undeca’) and the number ‘2’ by ‘do’ (except in the cases of ‘dicta’ and ‘dilia’). The numerical term for the number ‘11’ is ‘undeca’.

P-14.2.1.1.2 The prefix ‘mono’ is not used in systematically formed names to indicate the presence of one nomenclatural feature, for example suffixes, prefixes, endings. It is used in functional class nomenclature to designate a monoester of a diacid, for example phthalic acid monomethyl ester, and in terminology, to emphasize singleness, for example, monocyclic and mononuclear in contrast to bicyclic and polynuclear.

P-14.2.1.2 Derivation of basic numerical terms

After ‘undeca-’ (for the number eleven), composite numerical terms are formed systematically by citing the basic terms in the order opposite to that of the constituent digits in the arabic numbers. The composite terms are formed by direct joining of the basic terms, without hyphen(s). The letter ‘i’ in ‘icosa’ is elided after a vowel.

Examples:

486 hexaoctacontatetracta
| 6 | 80 | 400 |

14	tetradeca	21	henicosa	22	docosa

23	tricosa	24	tetracosa	41	hentetraconta
52	dopentaconta	111	undecahecta	363	trihexacontatricta

P-14.2.2 Numerical terms for compound or complex features

Multiplicative prefixes for compound or complex entities, such as substituted substituents, are formed by adding the ending ‘kis’ to the basic multiplicative prefix ending in ‘a’, ‘tetrakis’, ‘pentakis’, etc. (ref. 15). The prefixes ‘bis’ and ‘tris’ correspond to ‘di’ and ‘tri’. The basic prefix ‘mono’ has no counterpart in this series.

Examples:

2	bis	3	tris	4	tetrakis
231	hentriacontadictakis				

P-14.2.3 Multiplicative prefixes for naming assemblies of identical units

The traditional prefixes used to denote the number of repeated identical units in unbranched ring assemblies (see P-28) are as follows:

2	bi	5	quinque	8	octi
3	ter	6	sexi	9	novi
4	quater	7	septi	10	deci

This list has been completed from 11 to 9999. The prefixes are formed by changing the ending ‘a’ of basic numerical prefixes into ‘i’, for example, ‘undeci’ for the number ‘11’, ‘hexadeci’ for the number ‘16’, ‘tetraconti’ for the number ‘40’.

P-14.3 LOCANTS

P-14.3.1 Types of locants

Traditional types of locants are arabic numbers, for example, 1, 2, 3; primed locants, for example, 1′, 1‴, 2″; locants including a lower case Roman letter, for example, 3a, 3b; italicized Roman letters, for example, *O*, *N*, *P*; Greek letters, for example, ‘α-, β-, γ-’ and compound locants, for example, ‘1(10)’ and ‘5(17)’.

The locants *o*, *m*, *p* are no longer recommended; the numerical locants ‘1,2-’, ‘1,3-’, and ‘1,4-’ must be used in substitutive names. However, as an exception, the three isomers of xylene and cresol are still recognized as *o*-, *m*-, and *p*-xylene and *o*-, *m*-, and *p*-cresol in general IUPAC nomenclature (see P-22.1.3 and P-63.1.1.2). The prefixes *o*-, *m*-, and *p*-tolyl are still recognized for general nomenclature (see P-29.6.2.3). No substitution is allowed.

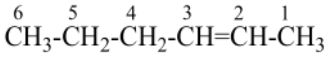
Composite locants, for example, 3^2, $2a^1$, $N^{2'}$, and O^3 have been developed in recent years for various purposes and are included in these recommendations. They are used in phane nomenclature to indicate positions in amplificants (see P-26.4.3); for numbering in ring assemblies (see P-28.3); to denote interior positions in fused ring systems (see P-25.3.3.3); and in von Baeyer descriptors for spiro ring systems (see P-24.2.2). They are also used in steroid (ref. 16 and P-101.7.1.1), tetrapyrrole (ref. 17), and amino acid and peptide nomnclature (ref. 18 and P-103.2.1)).

Primes are added to differentiate between the same locant in the same or different parts of the structure, for example, 1′, 2″, *N*′, and α′. In locants consisting of two or more characters, primes are generally added to the primary character. For example, in locants including a lower case Roman letter, used in fused rings, primes are added following the arabic number, for example, 3′a and $2'a^1$; this format follows the principle that in locants for fusion positions in a fused ring system a letter follows the previous peripheral locant. For composite locants used in phane nomenclature, the prime follows the superatom locant, as in $2'^3$ and $2'^{4a}$. In multiplicative nomenclature, primes may appear just after a letter locant, such as N'^4 or following the composite letter locant, such as $N^{2'}$.

P-14.3.2 Position of locants

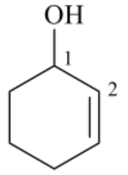
Locants (numerals and/or letters) are placed immediately before that part of the name to which they relate, except in the case of the traditional contracted names when locants are placed at the front of their names.

Examples:

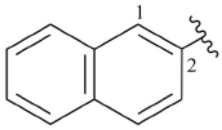


$$\overset{6}{C}H_3\text{-}\overset{5}{C}H_2\text{-}\overset{4}{C}H_2\text{-}\overset{3}{C}H{=}\overset{2}{C}H\text{-}\overset{1}{C}H_3$$

hex-2-ene (PIN)
(not 2-hexene)



cyclohex-2-en-1-ol (PIN)
(not 2-cyclohexen-1-ol)



naphthalen-2-yl (preferred prefix)
2-naphthyl (contracted name)
(not naphth-2-yl)

P-14.3.3 Citation of locants

In preferred IUPAC names, if any locants are essential for defining the structure of the parent structure or of a unit of structure as defined by its appropriate enclosing marks, then all locants must be cited for the parent structure or that structural unit. For example, the omission of the locant '1' in 2-chloroethanol, while permissible in general usage, is not allowed in preferred IUPAC names, thus the name 2-chloroethan-1-ol is the PIN. And in the following example, 1-phenyl-2-(phenyldiazenyl)-2-(phenylhydrazinylidene)ethan-1-one (PIN), locants are not used for the structural units defined by the parentheses even though locants are used for these substituents of the parent structure ethanone. Also, in preferred IUPAC multiplicative names and in preferred IUPAC names for ring assemblies locants are always cited, e.g., 1,1′-oxydibenzene (P-15.3.1.3) and 1,1′-biphenyl (P-28.2.1). For omission of locants from a PIN see P-14.3.4.

P-14.3.4 Omission of locants

The practice of omitting locants when there is no ambiguity is widespread. However, for absolute clarity in preferred IUPAC names it is necessary to be prescriptive about when omission of locants is permissible.

Locants are omitted in preferred IUPAC names in the following cases.

P-14.3.4.1 Terminal locants are not cited in names for mono- and dicarboxylic acids derived from acyclic hydrocarbons and their corresponding acyl halides, amides, hydrazides, nitriles, esters, aldehydes, amidines, amidrazones, hydrazidines, and amidoximes, when unsubstituted or substituted on carbon atoms.

Examples:

$HOOC\text{-}CH_2\text{-}CH_2\text{-}COOH$
butanedioic acid (PIN)

$HOOC\text{-}CH_2\text{-}CH(Cl)\text{-}COOH$
chlorobutanedioic acid (PIN)

$CH_3\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}CO–$
pentanoyl (preferred prefix)

$H_2N\text{-}CO\text{-}CH(CH_3)\text{-}CO\text{-}NH_2$
2-methylpropanediamide (PIN)

$CH_3\text{-}NH\text{-}CO\text{-}CH_2\text{-}CO\text{-}NH\text{-}CH_3$
N^1,N^3-dimethylpropanediamide (PIN)
(not N^1,N^3-dimethylpropane-1,3-diamide)

P-14.3.4.2 The locant '1' is omitted:

(a) in substituted mononuclear parent hydrides;

Examples:

CH_3Cl
chloromethane (PIN)

SiH_2Cl_2
dichlorosilane (from silane, a preselected name)

$(CH_3)_3Al$
trimethylalumane

(b) in monosubstituted homogeneous chains consisting of only two identical atoms;

Examples:

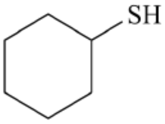
CH_3-CH_2-OH
ethanol (PIN)

NH_2-NH-Cl
chlorohydrazine (from hydrazine, a preselected name)

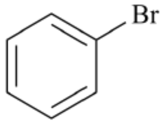
NH_2-NH–
hydrazinyl (preselected prefix) (not hydrazin-1-yl)

(c) in monosubstituted homogeneous monocyclic rings;

Examples:



cyclohexanethiol (PIN)



bromobenzene (PIN)

(d) in any dinuclear, unsubstituted alkenes and alkynes and monounsaturated cycloalkenes and cycloalkynes; similarly, in unsubstituted monounsaturated compounds composed of homogeneous chains containing elements of Groups 13, 14, 15, and 16, and corresponding monounsaturated cyclic compounds.

Examples:

CH_2=CH_2
ethene (PIN)

CH≡CH
acetylene (PIN)

CH_3-CH=CH_2
propene (PIN)

NH=NH
diazene (preselected name)

SiH≡SiH
disilyne (preselected name)

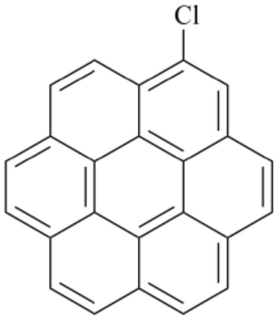
H_2N-N=NH
triazene (preselected name)

P-14.3.4.3 The locant is omitted in monosubstituted symmetrical parent hydrides or parent compounds where there is only one kind of substitutable hydrogen.

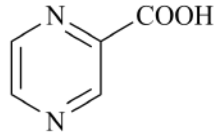
Examples:

CH_3-NH-CO-NH_2
methylurea (PIN)

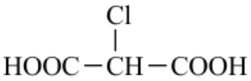
Cl-SiH_2-O-SiH_3
chlorodisiloxane (from disiloxane, a preselected name)



chlorocoronene (PIN)



pyrazinecarboxylic acid (PIN)



$$\mathrm{HOOC-\overset{\displaystyle Cl}{\overset{|}{C}}H-COOH}$$

chloropropanedioic acid (PIN)
chloromalonic acid

P-14.3.4.4 Locants are omitted when no isomer can be generated by moving suffixes and/or prefixes (if any) from their position to another or by interchanging them between two different positions.

Examples:

$\mathrm{CH_3\text{-}CH{=}N\text{-}NH}$–
ethylidenehydrazinyl (preferred prefix)
(not 2-ethylidenehydrazin-1-yl)

$\mathrm{HC{\equiv}Si\text{-}Si{\equiv}C\text{-}CH_3}$
ethylidyne(methylidyne)disilane
(not 1-ethylidyne-2-methylidynedisilane)

$\mathrm{C_6H_5\text{-}CH{=}SiH\text{-}Si({=}CH\text{-}C_6H_5)}$–
dibenzylidenedisilanyl (preferred prefix)
(not 1,2-dibenzylidenedisilan-1-yl)

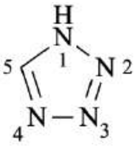
$\mathrm{H_2C{=}P\text{-}O\text{-}PH\text{-}O\text{-}P{=}CH\text{-}CH_3}$
ethylidene(methylidene)triphosphoxane (PIN)
(not 1-ethylidene-5-methylidenetriphosphoxane)

$\mathrm{H_2Si{=}N\text{-}NH\text{-}Cl}$
chloro(silylidene)hydrazine (preselected name)
(not 1-chloro-2-silylidenehydrazine)

$\mathrm{Br\text{-}S\text{-}S\text{-}CH_3}$
(bromodisulfanyl)methane (PIN)
(not bromo(methyl)disulfane see P-63.3.1;
not 1-bromo-2-methyldisulfane)

$\mathrm{O{=}C{=}CH}$–
oxoethenyl (preferred prefix)

$\mathrm{Cl\text{-}N{=}N}$–
chlorodiazenyl (preferred prefix)



1*H*-tetrazole (PIN)
(not 1*H*-1,2,3,4-tetrazole)

In the following examples locants are needed.

$CH_3\text{-}CH_2\text{-}CH{=}SiH\text{-}Si({=}CH\text{-}CH_3)\text{–}$
1-ethylidene-2-propylidenedisilan-1-yl (preferred prefix)
(by interchanging the two substituent groups another isomer
is generated, i.e., 2-ethylidene-1-propylidenedisilan-1-yl)

$CH_3\text{-}CH{=}SiH\text{-}SiH_2\text{-}Cl$
1-chloro-2-ethylidenedisilane (PIN)
(another isomer is generated by moving the Cl atom
to the other Si atom, i.e., 1-chloro-1-ethylidenedisilane)

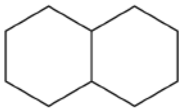
$Cl\text{-}CH{=}CH\text{–}$
2-chloroethen-1-yl (preferred prefix)
2-chlorovinyl

As an exception the locant is not omitted from propa-1,2-diene, propan-2-one, butan-2-one, prop-2-enoic acid and prop-2-ynoic acid although unambiguous without a locant.

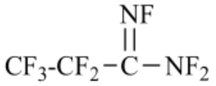
P-14.3.4.5 All locants are omitted in compounds or substituent groups in which all substitutable positions are completely substituted or modified, for example, by hydro, in the same way. Except for hydrogen atoms attached to chalcogen atoms, such as in acids, alcohols, and to the carbon atoms of formyl groups (aldehydes), all hydrogen atoms are considered substitutable.

In case of partial substitution or modification, all numerical prefixes must be indicated. The prefix ‘per-’ is no longer recommended.

Examples:



decahydronaphthalene (PIN)



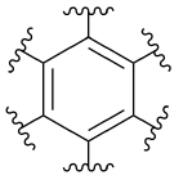
$$CF_3\text{-}CF_2\text{-}\overset{\overset{\displaystyle NF}{\|}}{C}\text{-}NF_2$$

octafluoropropanimidamide (PIN)

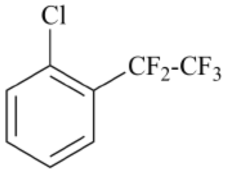
$$\overset{4}{C}F_3\text{-}\overset{3}{C}F_2\text{-}\overset{2}{C}F_2\text{-}\overset{1}{C}OOH$$

heptafluorobutanoic acid (PIN)

$CF_3\text{-}CF_2\text{-}CH_2\text{-}OH$
2,2,3,3,3-pentafluoropropan-1-ol (PIN)

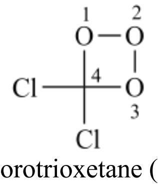


benzenehexayl (preferred prefix)



1-chloro-2-(pentafluoroethyl)benzene (PIN)

$F_2N\text{-}CO\text{-}NF_2$
tetrafluorourea (PIN)

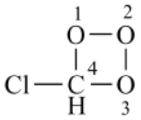


dichlorotrioxetane (PIN)

P-14.3.4.6 All locants are omitted for parent compounds when all substitutable hydrogen atoms have the same locant.

Examples:

$F_2CH\text{-}COOH$
difluoroacetic acid (PIN)
(not 2,2-difluoroacetic acid)



chlorotrioxetane (PIN)
(not 4-chloro-1,2,3-trioxetane)

P-14.3.5 Lowest set of locants

The lowest set of locants is defined as the set that, when compared term by term with other locant sets, each cited in order of increasing value, has the lowest term at the first point of difference; for example, the locant set ‘2,3,5,8’ is lower than ‘3,4,6,8’ and ‘2,4,5,7’.

Primed locants are placed immediately after the corresponding unprimed locants in a set arranged in ascending order; locants consisting of a number and a lower-case letter with or without primes as 4a and 4′a (not 4a′) are placed immediately after the corresponding numeric locant and are followed by locants having superscripts.

Italic capital and lower-case letter locants are lower than Greek letter locants, which, in turn, are lower than numerals.

Examples:

2 is lower than 2′
3 is lower than 3a
8a is lower than 8b
4′ is lower than 4a
4a is lower than 4′a
1^2 is lower than 1^3
1^4 is lower than 2′
3a is lower than $3a^1$
1,1,1,4,2 is lower than 1,1,4,4,2
1,1′,2′,1″,3″,1‴ is lower than 1,1′,3′,1″,2″,1‴
N,α,1,2 is lower than 1,2,4,6

Note: An exception must be noted in the field of carotenoid nomenclature, where 5,8,5′,8′- is used rather than 5,5′,8,8′- (see P-101.5.2); the latter would be recommended for systematic substitutive nomenclature

P-14.4 NUMBERING

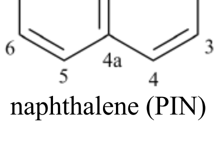
When several structural features appear in cyclic and acyclic compounds, low locants are assigned to them in the following decreasing order of seniority:

> Two important changes have been made to the 1979 recommendations (ref 1):
>
> (1) heteroatoms in chains are now considered to be a part of the parent hydride; as such, they have seniority over suffixes for numbering as for heteroatoms in rings;
>
> (2) hydro/dehydro prefixes are now classified as detachable prefixes but are not included in the category of alphabetized detachable prefixes; they are cited directly before the name of the parent hydride [see item (e) below].

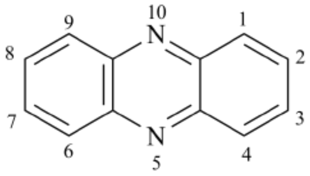
(a) fixed numbering in chains, rings, or ring systems, i.e., when the numbering of a system is fixed, for example in purine, anthracene, and phenanthrene, this numbering must be used, both in PINs and in general nomenclature;

Examples:

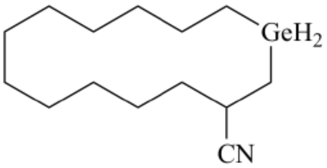
1 2 3 4 5 6 7 8 9 10 11 12 13 14
$CH_3\text{-}S\text{-}CH_2\text{-}CH_2\text{-}O\text{-}CH_2\text{-}CH_2\text{-}S\text{-}CH_2\text{-}CH_2\text{-}SiH_2\text{-}CH_2\text{-}CH_2\text{-}COOH$
5-oxa-2,8-dithia-11-silatetradecan-14-oic acid (PIN)



naphthalene (PIN)



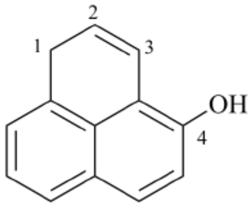
phenazine (PIN)



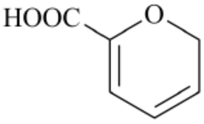
1-germacyclotetradecane-3-carbonitrile (PIN)

(b) indicated hydrogen for unsubstituted compounds; a higher locant may be needed at another position to accommodate a substituent suffix in accordance with structural feature (c);

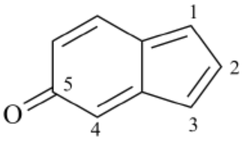
Examples:



1*H*-phenalen-4-ol (PIN)



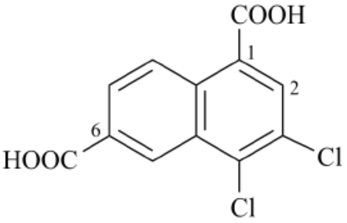
2*H*-pyran-6-carboxylic acid (PIN)



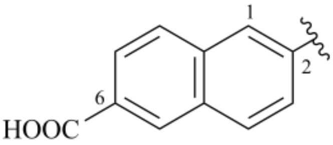
5*H*-inden-5-one (PIN)

(c) principal characteristic groups and free valences (suffixes);

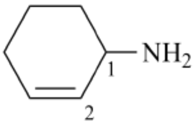
Examples:



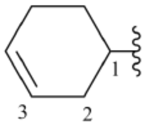
3,4-dichloronaphthalene-1,6-dicarboxylic acid (PIN)



6-carboxynaphthalen-2-yl (preferred prefix)



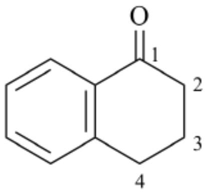
cyclohex-2-en-1-amine (PIN)



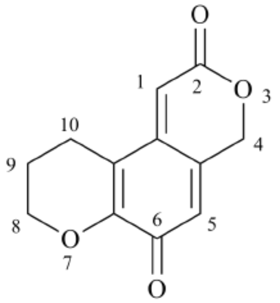
cyclohex-3-en-1-yl (preferred prefix)

(d) ‘added indicated hydrogen’ (consistent with the structure of the compound and in accordance with further substitution);

Examples:



3,4-dihydronaphthalen-1(2*H*)-one (PIN)



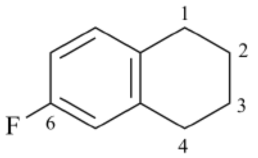
9,10-dihydro-2*H*,4*H*-benzo[1,2-*b*:4,3-*c*′]dipyran-2,6(8*H*)-dione (PIN)

(e) saturation/unsaturation:

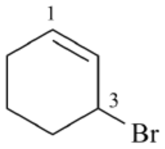
(i) low locants are given to hydro/dehydro prefixes (see first example and P-31.2.2) and ‘ene’ and ‘yne’ endings;

(ii) low locants are given first to multiple bonds as a set and then to double bonds (see second and third examples and P-31.1.1.1);

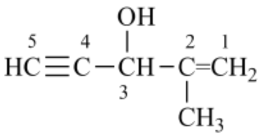
Examples:



6-fluoro-1,2,3,4-tetrahydronaphthalene (PIN)



3-bromocyclohex-1-ene (PIN)

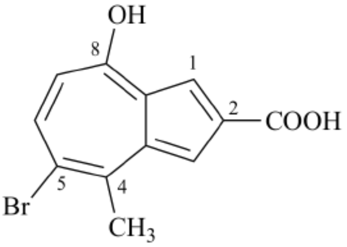


$$\overset{5}{H}C\equiv\overset{4}{C}-\underset{3}{\overset{OH}{CH}}-\underset{CH_3}{\overset{2}{C}}=\overset{1}{C}H_2$$

2-methylpent-1-en-4-yn-3-ol (PIN)
(not 4-methylpent-4-en-1-yn-3-ol)

(f) detachable alphabetized prefixes, all considered together in a series of increasing numerical order;

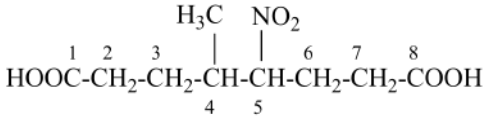
Example:



5-bromo-8-hydroxy-4-methylazulene-2-carboxylic acid (PIN)
(the locant set ‘4,5,8’ is lower than ‘4,7,8’)

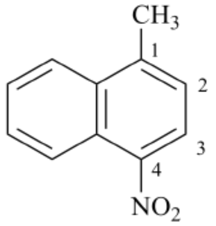
(g) lowest locants for the substituent cited first as a prefix in the name;

Examples:



$$\overset{1}{\mathrm{HOOC}}\text{-}\overset{2}{\mathrm{CH_2}}\text{-}\overset{3}{\mathrm{CH_2}}\text{-}\underset{4}{\overset{\mathrm{H_3C}}{\overset{|}{\mathrm{CH}}}}\text{-}\underset{5}{\overset{\mathrm{NO_2}}{\overset{|}{\mathrm{CH}}}}\text{-}\overset{6}{\mathrm{CH_2}}\text{-}\overset{7}{\mathrm{CH_2}}\text{-}\overset{8}{\mathrm{COOH}}$$

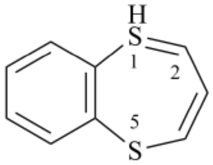
4-methyl-5-nitrooctanedioic acid (PIN)



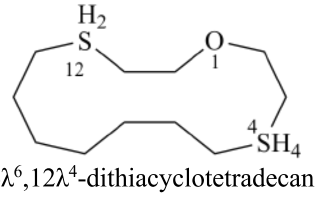
1-methyl-4-nitronaphthalene (PIN)
(not 4-methyl-1-nitronaphthalene)

(h) When a choice is needed between the same skeletal atom in different valence states, the one in a nonstandard valence state is assigned the lower locant. If a further choice is needed between the same skeletal atom in two or more nonstandard valence states, the one in the higher valence state is assigned the lower locant;

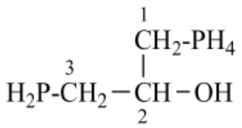
Examples:



1λ^4,5-benzodithiepine (PIN)



1-oxa-4λ^6,12λ^4-dithiacyclotetradecane (PIN)



$$\mathrm{H_2P\text{-}\overset{3}{CH_2}-\underset{2}{\overset{\overset{1}{CH_2\text{-}PH_4}}{\overset{|}{CH}}}-OH}$$

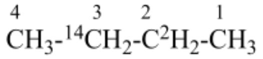
1-(λ^5-phosphanyl)-3-phosphanylpropan-2-ol (PIN)
(λ^5-phosphanyl is cited before phosphanyl and is given the lower locant)

(i) When there is a choice between equivalent numberings in an isotopically unmodified compound, the starting point and the direction of numbering of the analogous isotopically substituted compound are chosen so as to give lowest locants to the modified atoms or groups considered together as a set in increasing numerical order. If a choice still remains, the lower locant is given to the nuclide of higher atomic number. In the case of different nuclides of the same element, the lower locant is assigned to the nuclide of higher mass number;

Examples:

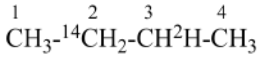
$$\overset{1}{\mathrm{CH_3}}\text{-}\overset{2}{\mathrm{{}^{14}CH_2}}\text{-}\overset{3}{\mathrm{CH_2}}\text{-}\overset{4}{\mathrm{CH_3}}$$

(2-^{14}C)butane (PIN)
[not (3-^{14}C)butane]



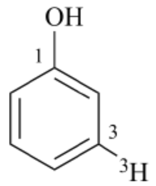
$\overset{4}{CH_3}\text{-}{}^{14}\overset{3}{C}H_2\text{-}\overset{2}{C}{}^{2}H_2\text{-}\overset{1}{C}H_3$

(3-^{14}C,2,2-^{2}H$_2$)butane (PIN)
[not (2-^{14}C,3,3-^{2}H$_2$)butane]

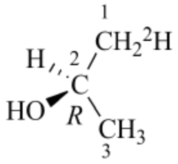


$\overset{1}{CH_3}\text{-}{}^{14}\overset{2}{C}H_2\text{-}\overset{3}{C}H{}^{2}H\text{-}\overset{4}{C}H_3$

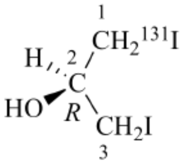
(2-^{14}C,3-^{2}H$_1$)butane (PIN)
[not (3-^{14}C,2-^{2}H$_1$)butane]



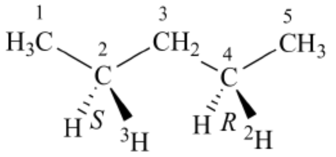
(3-^{3}H)phenol (PIN)



(2*R*)-(1-^{2}H$_1$)propan-2-ol (PIN)



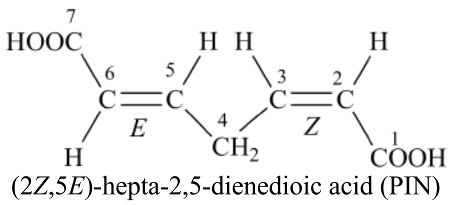
(2*R*)-1-(^{131}I)iodo-3-iodopropan-2-ol (PIN)
(see P-82.2.2.1)



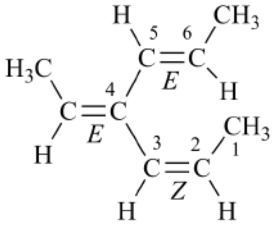
(2*S*,4*R*)-(4-^{2}H$_1$,2-^{3}H$_1$)pentane (PIN)
[not (2*R*,4*S*)-(2-^{2}H$_1$,4-^{3}H$_1$)pentane;
isotopic modifications have seniority for low locants over
stereodescriptors described in (j) below]

(j) When there is a choice for lower locants related to the presence of stereogenic centers or stereoisomers, the lower locant is assigned to CIP stereodescriptors *Z*, *R*, *M*, and *r* (pseudoasymmetry) that are preferred to *E*, *S*, *P*, and *s*, respectively, which are preferred to the non-CIP stereodescriptors *cis*, *trans*, or *r* (reference), *c*, and *t* (see P-91.2 for CIP and non-CIP stereodescriptors).

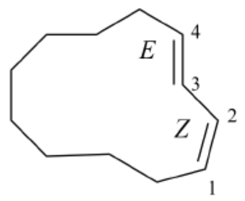
Examples:



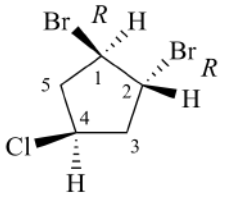
(2*Z*,5*E*)-hepta-2,5-dienedioic acid (PIN)
(the chain is numbered by assigning the low locant to the '*Z*' double bond)



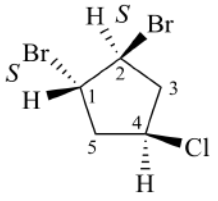
(2*Z*,4*E*,5*E*)-4-ethylidenehepta-2,5-diene (PIN)
(low locants are assigned to the longest chain, then to the '*Z*' double bond)



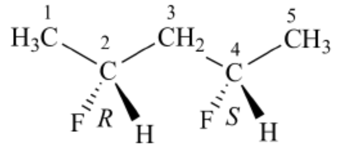
(1*Z*,3*E*)-cyclododeca-1,3-diene (PIN)


Br
R
H
Br
R
H
1
2
5
4
3
Cl
H

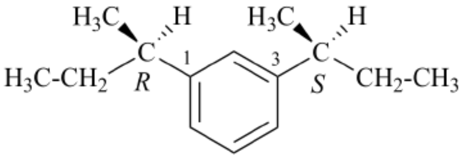
or


H
S
Br
Br
S
H
1
2
3
4
5
Cl
H

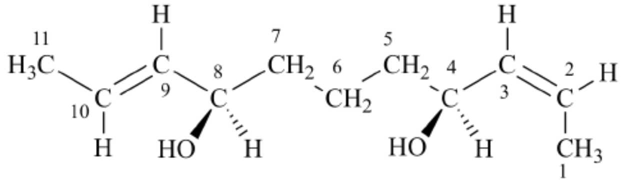
rel-(1*R*,2*R*)-1,2-dibromo-4-chlorocyclopentane (PIN)
1*r*,2*t*-dibromo-4*c*-chlorocyclopentane
(the preferred IUPAC name is denoted by CIP stereodescriptors;
in the second name, the relative configuration is expressed by the
non-CIP stereodescriptors ‘1*r*,2*t*,4*c*’ rather than ‘1*r*,2*t*,4*t*’,
because a ‘*cis*’ arrangement, denoted by ‘*c*’, has priority
over a ‘*trans*’ arrangement, denoted by ‘*t*’, in position ‘4’)


1
3
5
H3C
2
CH2
4
CH3
C
C
F
R
H
F
S
H

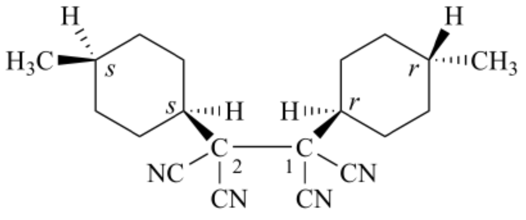
(2*R*,4*S*)-2,4-difluoropentane (PIN)


H3C
H
H3C
H
C
1
3
C
H3C-CH2
R
S
CH2-CH3

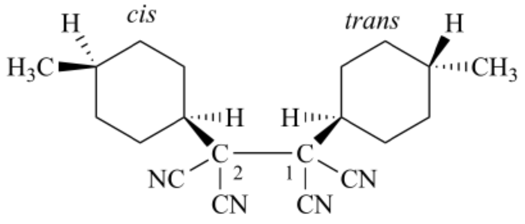
1-[(2*R*)-butan-2-yl]-3-[(2*S*)-butan-2-yl]benzene (PIN)


H
H
11
7
5
H3C
C
8
CH2
6
CH2
4
C
2
H
9
3
10
C
C
CH2
C
C
H
HO
H
HO
H
CH3
1

(2*Z*,4*S*,8*R*,9*E*)-undeca-2,9-diene-4,8-diol (PIN)
(the choice is between ‘*E*’ and ‘*Z*’ for position ‘2’, not between ‘*R*’ and ‘*S*’ for position ‘4’)

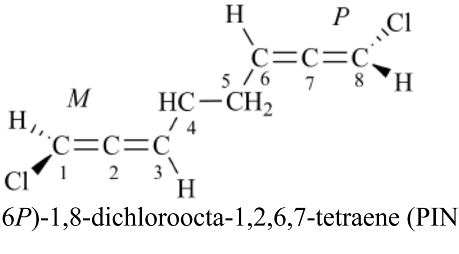

H
H
H3C
s
r
CH3
s
H
H
r
C
C
NC
2
1
CN
CN
CN

I


H
cis
trans
H
H3C
CH3
H
H
C
C
NC
2
1
CN
CN
CN

II

(**I**) 1-[(1*r*,4*r*)-4-methylcyclohexyl]-2-[(1*s*,4*s*)-4-methylcyclohexyl]ethane-1,1,2,2-tetracarbonitrile (PIN)
(the substituent denoted by the ‘*r*’ stereodescriptor receives the lowest locant, ‘1’;
the use of CIP stereodescriptors generates the preferred IUPAC name)
(**II**) 1-(*cis*-4-methylcyclohexyl)-2-(*trans*-4-methylcyclohexyl)ethane-1,1,2,2-tetracarbonitrile
(the ‘*cis*’ substituent receives the lowest locant, ‘1’)


H
P
Cl
C=C=C
5
6
7
8
H
M
HC
CH2
4
H
C=C=C
Cl
1
2
3
H

(1*M*,6*P*)-1,8-dichloroocta-1,2,6,7-tetraene (PIN)

P-14.5 ALPHANUMERICAL ORDER

Alphanumerical order has been commonly called ‘alphabetical order’. As these ordering principles do involve ordering both letters and numbers, in a strict sense, it is best called ‘alphanumerical order’ in order to convey the message that both letters and numbers are involved.

Alphanumerical order is used to establish the order of citation of detachable substituent prefixes (not the detachable saturation prefixes, hydro and dehydro), and the numbering of a chain, ring, or ring system when a choice is possible.

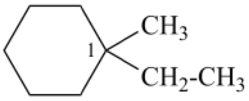
Alphanumerical order is applied as follows in organic nomenclature. Nonitalic Roman letters are considered first, unless used as locants or part of a compound or composite locant, for example, ‘*N*’ or ‘4a’ (see P-14.3), or in an isotopic descriptor. When all the Roman letters are identical, the set of locants for all initial locants for primary substituents, that is, locants appearing ahead of the first Roman letter of each primary substituent, are compared. Absence of locants is most preferred, followed by italic Roman letter locants, Greek letter locants (as in conjunctive names), if any, and arabic numerals in order from lowest to highest. Thus, the preferred order for alphanumerical order is: nonitalic Roman letters > italic letters > Greek letters.

For the sorting of nonalphanumerical characters, see P-14.6.

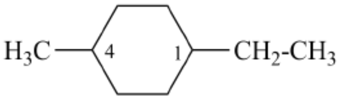
In these subsections the principles of alphanumerical order do not include Greek letters (except in conjunctive names) or isotopic or stereochemical descriptors.

P-14.5.1 Simple prefixes (i.e., those describing atoms and unsubstituted substituents) are arranged alphabetically; multiplicative prefixes, if necessary, are then inserted and do not alter the alphabetical order already established.

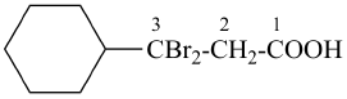
Examples:



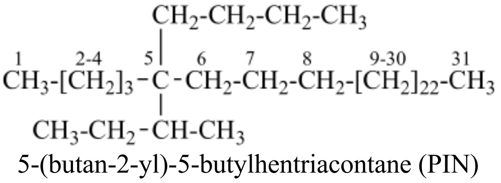
1-ethyl-1-methylcyclohexane (PIN)



1-ethyl-4-methylcyclohexane (PIN)
[for numbering, see P-14.4 (g)]

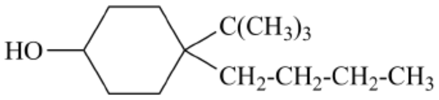


3,3-dibromo-3-cyclohexylpropanoic acid (PIN)
(not 3-cyclohexyl-3,3-dibromopropanoic acid)

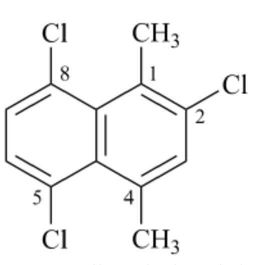


$$\overset{1}{CH_3}\text{-}\overset{2\text{-}4}{[CH_2]_3}\text{-}\overset{5}{\underset{CH_3\text{-}CH_2\text{-}CH\text{-}CH_3}{\overset{CH_2\text{-}CH_2\text{-}CH_2\text{-}CH_3}{C}}}\text{-}\overset{6}{CH_2}\text{-}\overset{7}{CH_2}\text{-}\overset{8}{CH_2}\text{-}\overset{9\text{-}30}{[CH_2]_{22}}\text{-}\overset{31}{CH_3}$$

5-(butan-2-yl)-5-butylhentriacontane (PIN)
[butyl is not treated as butan-1-yl; for the use of enclosing marks, see P-16.5.1.2]



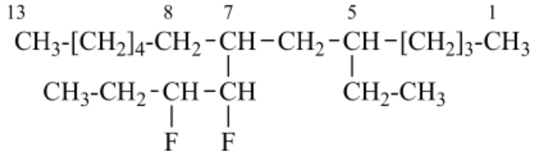
4-butyl-4-*tert*-butylcyclohexan-1-ol (PIN)



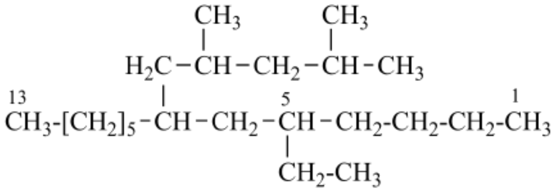
2,5,8-trichloro-1,4-dimethylnaphthalene (PIN)
[not 1,4-dimethyl-2,5,8-trichloronaphthalene;
‘trichloro’ is cited before ‘dimethyl’ as ‘chloro’ is earlier alphabetically than ‘methyl’]
[not 1,4,6-trichloro-5,8-dimethylnaphthalene;
the locant set ‘1,2,4,5,8’ is lower than ‘1,4,5,6,8’ (see P-14.3.5)]

P-14.5.2 The name of a prefix for a substituent is considered to begin with the first letter of its complete name.

Examples:



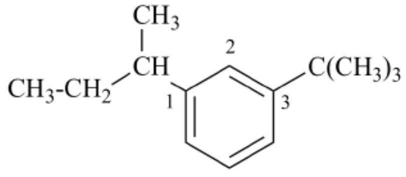
7-(1,2-difluorobutyl)-5-ethyltridecane (PIN)
[not 5-ethyl-7-(1,2-difluorobutyl)tridecane;
the compound substituent name in the PIN starts with ‘d’, and ‘d’ is earlier alphabetically than ‘e’]



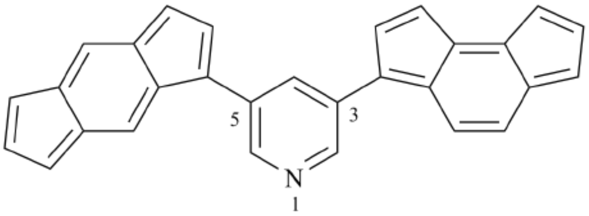
7-(2,4-dimethylpentyl)-5-ethyltridecane (PIN;
(‘dimethylpentyl’ begins with ‘d’ that precedes ‘e’ in alphabetical order)

P-14.5.3 When an alphanumerical ordering is required and Roman letters do not permit a decision for the order of citation, italicized letters are considered.

Examples:



3-*tert*-butyl-1-(1-methylpropyl)benzene
1-(butan-2-yl)-3-*tert*-butylbenzene (PIN)
(for use of enclosing marks, see P-16.5.1.2)
[not 1-*sec*-butyl-3-*tert*-butylbenzene]

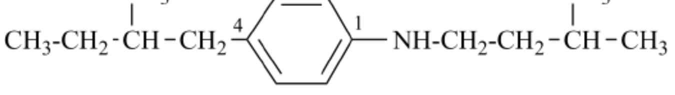


3-(*as*-indacen-3-yl)-5-(*s*-indacen-1-yl)pyridine (PIN)
[not 5-*s*-indacen-1-yl-3-*as*-indacen-3-ylpyridine]

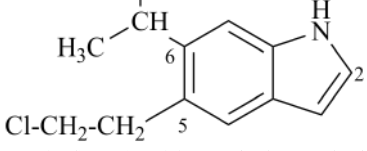
And similarly, naphtho[1,2-*f*]quinolin-2-yl is alphanumerically preferred to naphtho[1,2-*g*]quinolin-1-yl (‘f’ before ‘g’).

P-14.5.4 When two or more prefixes consist of identical Roman letters, priority for order of citation is given to the group that contains the lowest locant(s) at the first point of difference.

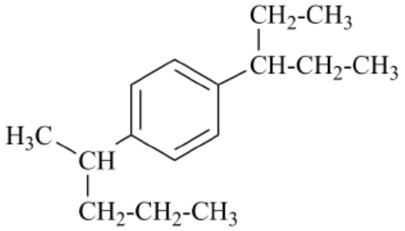
Examples:



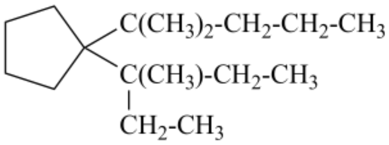
4-(2-methylbutyl)-*N*-(3-methylbutyl)aniline (PIN)
4-(2-methylbutyl)-*N*-(3-methylbutyl)benzenamine
(for ordering the substituents ‘2’ is lower than ‘3’;
the fact that ‘*N*’ is lower than ‘4’ is irrelevant)



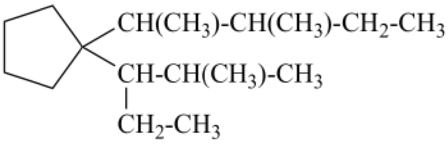
6-(1-chloroethyl)-5-(2-chloroethyl)-1*H*-indole (PIN)
(the locant ‘1’ is lower than ‘2’)



1-(pentan-2-yl)-4-(pentan-3-yl)benzene (PIN)
(the locant ‘2’ is lower than ‘3’; for the use of enclosing marks, see P-16.5.1.2)



1-(2-methylpentan-2-yl)-1-(3-methylpentan-3-yl)cyclopentane (PIN)
[not 1-(3-methylpentan-3-yl)-1-(2-methylpentan-2-yl)cyclopentane;
the locant set ‘2,2’ is lower than ‘3,3’)



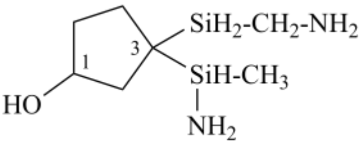
1-(2-methylpentan-3-yl)-1-(3-methylpentan-2-yl)cyclopentane (PIN)
[not 1-(3-methylpentan-2-yl)-1-(2-methylpentan-3-yl)cyclopentane;
the locant set ‘2,3’ is lower than ‘3,2’]

P-14.6 NONALPHANUMERICAL ORDER

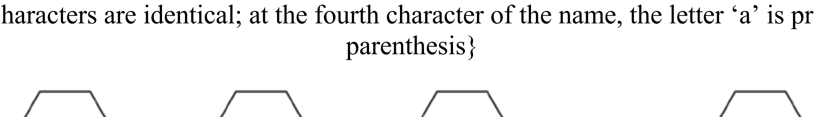
Alphanumerical ordering resolves practically all of the ordering problems for organic names. However, there are the occasional names in which the alphanumerical character numberings are identical. In such cases, other characters, such as enclosing marks or punctuation marks, must be compared with letters and/or numbers, or with each other to select a preferred IUPAC name. Letters or numbers are always preferred to any other character. When necessary the order of priority for other characters is as follows, listed in decreasing priority order: braces > square brackets > parentheses (round brackets) > periods > commas > semi-colons > colons > hyphens.

Note: Previous recommendations did not provide rules for selection of a preferred name beyond the ordering alphanumerical characters. For compounds whose alphanumerical charactericts do not lead to a unique name, an ordering for nonalphanumerical characters, such as commas, enclosing marks, etc., is needed. The above paragraph provides this information.

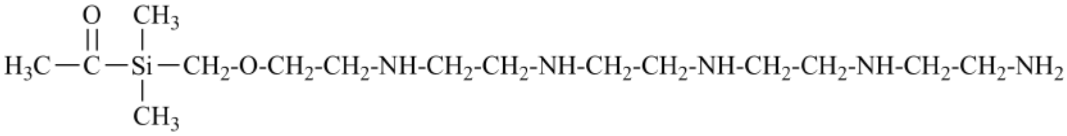
Examples:



3-[amino(methyl)silyl]-3-[(aminomethyl)silyl]cyclopentan-1-ol (PIN)
{not 3-[(aminomethyl)silyl]-3-[amino(methyl)silyl]cyclopentan-1-ol;
alphanumerical characters are identical; at the fourth character of the name, the letter ‘a’ is preferred to an open parenthesis}



1-[(cyclohexylmethoxy)methyl]-4-{[4-(cyclohexylmethyl)cyclohexyl]methyl}cyclohexane (PIN)
{not 1-({4-[(cyclohexylmethoxy)methyl]cyclohexyl}methyl)-4-(cyclohexylmethyl)cyclohexane
the alphabetic letters and the primary substituent locants are identical for both names;
however, there is no locant for the first internal substituent in the PIN, but in the
alternative name the locant for the first internal substituent is ‘4’ and no locant is preferred to ‘4’}



$H_3C-C(=O)-Si(CH_3)_2-CH_2-O-CH_2-CH_2-NH-CH_2-CH_2-NH-CH_2-CH_2-NH-CH_2-CH_2-NH-CH_2-CH_2-NH_2$

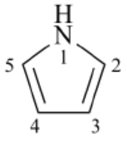
N^1-{2-[(acetyldimethylsilyl)methoxy]ethyl}-*N*^{2}-[2-({2-[(2-aminoethyl)amino]ethyl}amino)ethyl]ethane-1,2-diamine
N^1-[2-({2-[(acetyldimethylsilyl)methoxy]ethyl}amino)ethyl]-*N*^{2}-{2-[(2- aminoethyl)amino]ethyl}ethane-1,2-diamine
[the parent structure must be a diamine; alphanumerical orders of the first two names are the same;

at the third character the nonalphanumerical '{' is preferred to '['
19-amino-3,3-dimethyl-5-oxa-8,11,14,17-tetraaza-3-silanonadecan-2-one (PIN)

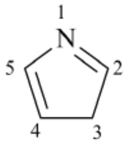
P-14.7 INDICATED AND 'ADDED INDICATED HYDROGEN'

P-14.7.1 Indicated hydrogen. Under certain circumstances it is necessary to indicate in the name of a mancude ring or ring system, i.e., one that contains the maximum number of noncumulative double bonds, one or more positions where no multiple bond is attached. When these positions are occupied by hydrogen atoms, the name can be made specific by indicating the position of one or more hydrogen atoms in the structure; this is accomplished by adding to the front of the name an italic capital '*H*' preceded by an appropriate numerical locant for each of these atoms.

Examples:



1*H*-pyrrole (PIN)
pyrrole



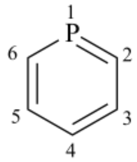
3*H*-pyrrole (PIN)

In the first example, the 'indicated hydrogen' locates one hydrogen atom in position '1' of the pyrrole ring; and in the second, the 'indicated hydrogen' indicates an 'extra' hydrogen atom at position '3' , i.e., one hydrogen atom more than the number present if there were a double bond in the ring at that position. Indicated hydrogen of this type precedes the name of a parent hydride. In general nomenclature, indicated hydrogen may be omitted (see P-25.7.1.3) and 1*H*-pyrrole can be called just 'pyrrole'. However, in a preferred IUPAC name a locant and the symbol '*H*' must be cited.

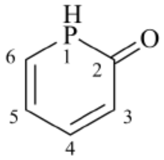
Detailed procedures for using 'indicated hydrogen' are discussed in P-58.2.1.

P-14.7.2 'Added indicated hydrogen'. A second type of indicated hydrogen is called 'added indicated hydrogen'. It describes hydrogen atoms added to a specified structure as the consequence of the addition of a suffix describing a structural modification. 'Added indicated hydrogen' is cited in parentheses after the locant of the structural feature to which it refers.

Example:



phosphinine (PIN)

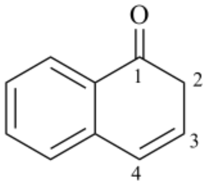


phosphinin-2(1*H*)-one (PIN)

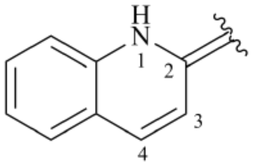
'Added indicated hydrogen' is used to introduce a free valence, a radical or an ionic center, or a principal characteristic group into a fully unsaturated heteromonocyclic compound or fused polycyclic system in the absence of, or lack of, sufficient hydrogen atoms to accommodate the operation at the site of the operation. Such substituted compounds are named by using a suffix to denote an operation on either a –CH= group or a =C< atom, or on equivalent heteroatoms such as –N=, or groups such as =NH.

Detailed procedures for using 'added indicated hydrogen' are discussed in P-58.2.2.

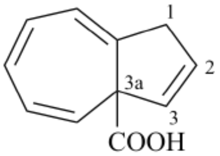
Examples:

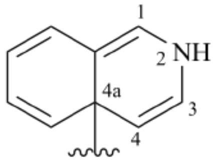


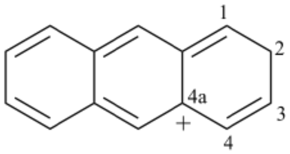
naphthalen-1(2*H*)-one (PIN)



quinolin-2(1*H*)-ylidene (preferred prefix)

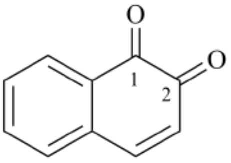

azulene-3a(1*H*)-carboxylic acid (PIN)

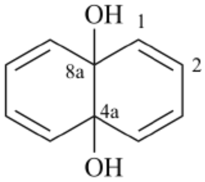

isoquinolin-4a(2*H*)-yl (preferred prefix)


anthracen-4a(2*H*)-ylium (PIN)

'Added indicated hydrogen' is not cited for preferred IUPAC names when two identical characteristic groups that essentially remove one of the double bonds of the parent structure are cited as suffixes in a mancude compound.

Examples:


naphthalene-1,2-dione (PIN)


naphthalene-4a,8a-diol (PIN)

P-14.8 ADDUCTS

P-14.8.1 Organic adducts

An adduct is a chemical species, each molecular entity of which is formed by direct combination of separate molecular entities in such a way that there may be a change of connectivity but no loss of atoms from any of the molecular entities (see ref. 19).

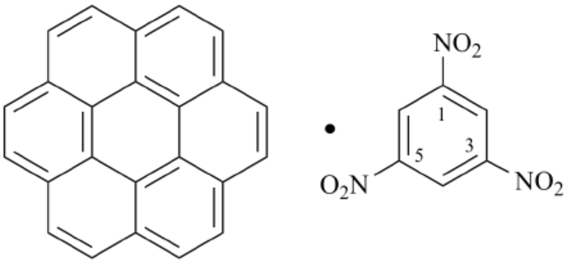
In this subsection, only adducts formed from organic compounds are considered. Inorganic adducts are discussed in ref. 12, IR-5.5. In this subsection, preferred IUPAC names for two different types of organic adducts are considered, Lewis adducts and π-adducts. Salts of organic bases or acids of unknown structure are named in a similar manner, for which see Chapter P-7. In general nomenclature the definition of an adduct as given above may include other types of representations as adducts, for example, butadiene—hydrogen chloride.

Formulas for these adducts are written in the order that follows the general seniority of organic compounds given in P-41. Names are formed by citing the names of individual compounds in the order of the formula connected by long (em) dashes (—). The proportions of components are indicated after the name by an arabic number separated by a solidus from other numbers; arabic numbers and the solidus are placed in parentheses, separated from the name by a space.

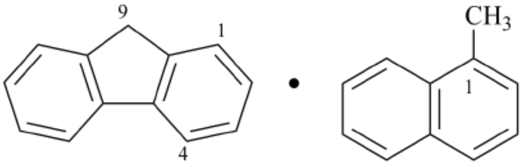
Salts and Lewis adducts between boron compounds and the Group 15 elements in which the mode of attachment is specified by italic element symbols are considered in P-68.1.6.

For adducts composed solely of organic compounds, the individual components are cited in the order of seniority of classes (see P-41) in formulas, no longer according to the number of species in the adduct, nor in accordance with the alphanumerical order as recommended in the 1979 Recommendations (see Rule D-1.55, ref. 1) and in the revised *Nomenclature of Inorganic Chemistry, 2005 Recommendations* (ref. 12). For adducts composed of organic and inorganic compounds, organic compounds precede inorganic compounds in formulas. Names are formed by citing the names of individual components in the order of the formula. The use of order of seniority, a universal system, as a ranking criterion is preferred to the language-dependent alphanumerical order for both preferred IUPAC names and in general nomenclature.

Examples:

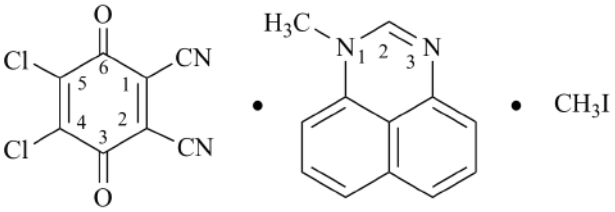

•
NO$_2$
1
5
3
O$_2$N
NO$_2$

coronene—1,3,5-trinitrobenzene (1/1) (PIN)

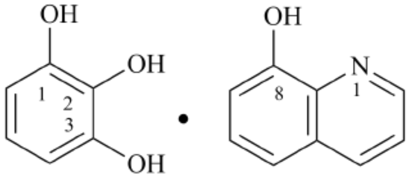


9*H*-fluorene—1-methylnaphthalene (1/1) (PIN)

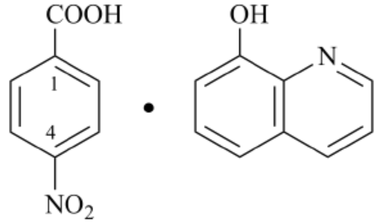
(HOOC-CH$_2$-NH-[CH$_2$]$_2$)$_2$N-CH$_2$-COOH • HN[CH$_2$-P(O)(OH)$_2$]$_2$ • H$_2$N-[CH$_2$]$_2$-NH$_2$
2,2′-{[(carboxymethyl)azanediyl]bis(ethane-2,1-diylazanediyl)}diacetic acid—[azanediylbis(methylene)]bis(phosphonic acid)—ethane-1,2-diamine (1/1/1)
N,*N*′-{[(carboxymethyl)azanediyl]di(ethan-2,1-diyl)}diglycine—[azanediylbis(methylene)]bis(phosphonic acid)—ethane-1,2-diamine (1/1/1)


O
Cl
CN
6
5
1
4
2
3
Cl
CN
O
•
H$_3$C
N
1
2
3
N
•
CH$_3$I

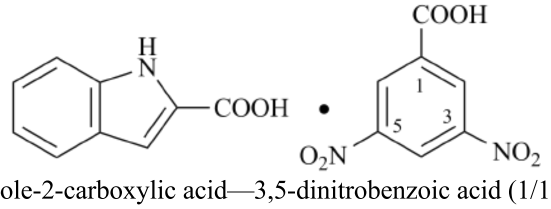
4,5-dichloro-3,6-dioxocyclohexa-1,4-diene-1,2-dicarbonitrile—1-methyl-1*H*-perimidine—iodomethane (1/1/1) (PIN)


OH
OH
1
2
3
OH
•
OH
N
8
1

benzene-1,2,3-triol—quinolin-8-ol (1/2) (PIN)

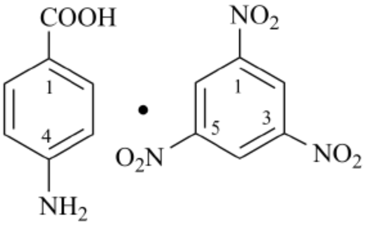

COOH
1
4
NO$_2$
•
OH
N

4-nitrobenzoic acid—quinolin-8-ol (1/1) (PIN)

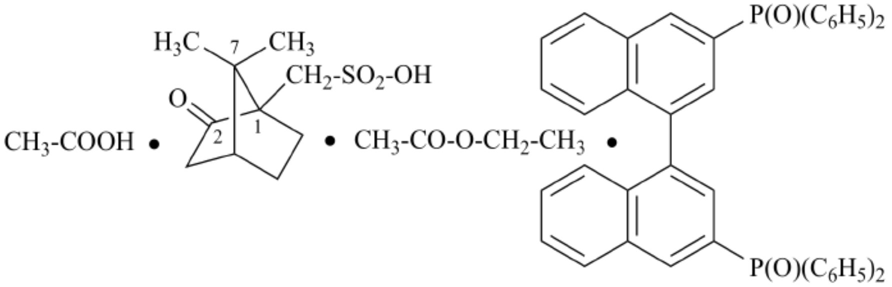

H
N
COOH
•
COOH
1
5
3
O$_2$N
NO$_2$

1*H*-indole-2-carboxylic acid—3,5-dinitrobenzoic acid (1/1) (PIN)

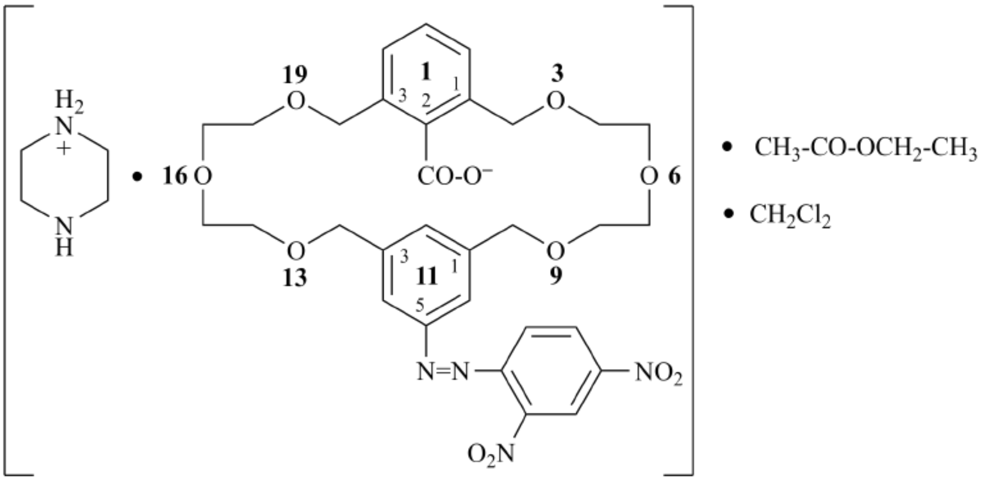
(C$_5$H$_5$)Fe(C$_5$H$_4$-CHO) • C$_6$H$_6$ • CBr$_4$
ferrocenecarbaldehyde—benzene—tetrabromomethane (1/1/1)



4-aminobenzoic acid—1,3,5-trinitrobenzene (1/1) (PIN)



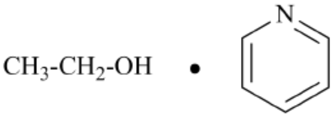
acetic acid—(7,7-dimethyl-2-oxobicyclo[2.2.1]heptan-1-yl)methanesulfonic acid—ethyl acetate—[1,1′-binaphthalene]-3,3′-diylbis(diphenyl-λ^5-phosphanone) (1/1/1/1) (PIN)



{piperazin-1-ium 11^5-[(2,4-dinitrophenyl)diazenyl]-3,6,9,13,16,19-hexaoxa-1,11(1,3)-dibenzenacycloicosaphane-1^2-carboxylate}—ethyl acetate—dichloromethane (1/1/1) (PIN)
{piperazin-1-ium 13-[(2,4-dinitrophenyl)azo]-3,6,9,17,20,23-hexaoxatricyclo[23.3.1.$1^{11,15}$]triaconta-1(29),11(30),12,14,25,27-hexaene-29-carboxylate}—ethyl acetate—dichloromethane (1/1/1)

Solvates, including hydrates (see P-14.8.2), are treated as adducts and preferred IUPAC names must use the notation for denoting the proportion of components described above. In general nomenclature, hydrates may be named by adding the words ‘hydrate’ to the name preceded by an appropriate numerical prefix, such as ‘mono’,‘di’, ‘tri’, etc. Terms such as ‘hemi’ and ‘sesqui’ are also used.

Example:



ethanol—pyridine (1/1) (PIN)

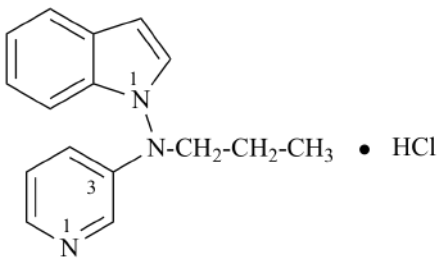
P-14.8.2 Mixed organic – inorganic adducts

Formulas for mixed adducts composed of organic and inorganic chemical species are written in the following order: organic components in order as described in P-14.8.1, inorganic components in order as described in Ref 12; water (if present), is cited last.

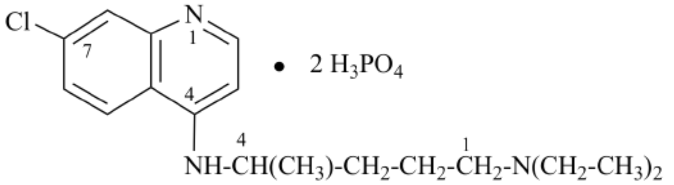
Although organic components are preferred IUPAC names, preferred IUPAC names cannot be assigned to mixed adducts because preferred IUPAC names have not yet been determined for inorganic components.

However, names are formed by citing the names of individual compounds, connected by long (em) dashes (—). The proportions of the components are indicated after the name by an arabic number(s) separated by a solidus enclosed in parentheses and separated from the name by a space. Hydrates may be named by adding the word ‘hydrate’ to the name preceded by an appropriate numerical prefix, such as ‘mono’,‘di’, ‘tri’, etc. Terms such as ‘hemi’ and ‘sesqui’ are also used.

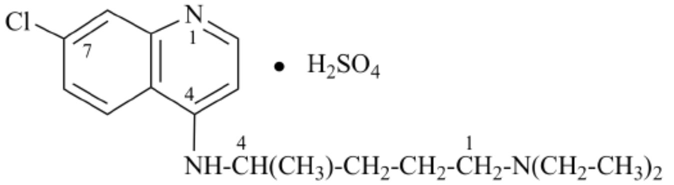
Examples:


1
N
N-CH2-CH2-CH3 • HCl
3
1
N

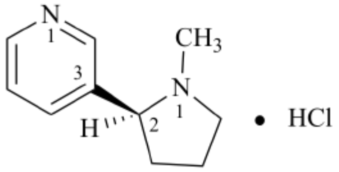
N-propyl-*N*-(pyridin-3-yl)-1*H*-indol-1-amine—hydrogen chloride (1/1)


Cl
N
1
7
4
• 2 H3PO4
4
1
NH-CH(CH3)-CH2-CH2-CH2-N(CH2-CH3)2

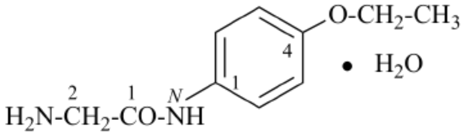
N^4-(7-chloroquinolin-4-yl)-*N*^{1},*N*^{1}-diethylpentane-1,4-diamine—phosphoric acid (1/2)


Cl
N
1
7
4
• H2SO4
4
1
NH-CH(CH3)-CH2-CH2-CH2-N(CH2-CH3)2

N^4-(7-chloroquinolin-4-yl)-*N*^{1},*N*^{1}-diethylpentane-1,4-diamine—sulfuric acid (1/1)

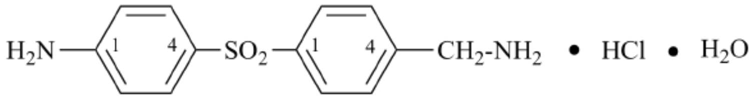

N
1
3
CH3
N
1
H
2
• HCl

3-[(2*S*)-1-methylpyrrolidin-2-yl]pyridine—hydrogen chloride (1/1)


O-CH2-CH3
4
• H2O
1
2
1
N
H2N-CH2-CO-NH

2-amino-*N*-(4-ethoxyphenyl)acetamide—water (1/1)
2-amino-*N*-(4-ethoxyphenyl)acetamide monohydrate

$HOOC\text{-}COOH \bullet H_2N\text{-}CH_2\text{-}CH_2\text{-}NH_2 \bullet 3/2\ H_2O$
oxalic acid—ethane-1,2-diamine—water (2/2/3)
oxalic acid—ethane-1,2-diamine sesquihydrate


H2N
1
4
SO2
1
4
CH2-NH2 • HCl • H2O

4-[4-(aminomethyl)benzene-1-sulfonyl]aniline—hydrogen chloride—water (1/1/1)

P-15 TYPES OF NOMENCLATURE

P-15.0 Introduction
P-15.1 Substitutive nomenclature
P-15.2 Functional class nomenclature
P-15.3 Multiplicative nomenclature
P-15.4 Skeletal replacement (‘a’) nomenclature
P-15.5 Functional replacement nomenclature
P-15.6 Conjunctive nomenclature

P-15.0 INTRODUCTION

‘Nomenclature’, in chemistry, is a system by which names are formed using various nomenclatural operations in accordance with a set of principles, rules, and conventions. There are fundamentally two types of nomenclature: (1) substitutive nomenclature, the principal nomenclature used in organic chemistry and the basis of IUPAC preferred organic names; and (2) additive nomenclature used in inorganic chemistry for generating coordination names. These two types are applied to name organic compounds and inorganic compounds, thus making nomenclature a matter of choice between them. For example, $SiCl_4$ can be named silicon tetrachloride (binary name), tetrachloridosilicon (coordination name), and tetrachlorosilane (substitutive name). Although coordination nomenclature is not discussed in these recommendations, it is used in the nomenclature of organometallic compounds belonging to Groups 1 and 2, for example, dimethylmagnesium. Binary names are used for salts composed of an anionic or cationic organic part, for example sodium acetate and methanaminium chloride. Preferred IUPAC names are recommended when there is a choice within the limits of the nomenclature of organic compounds, for example a choice between two substitutive names (acetic acid and ethanoic acid), between a multiplicative name and a substitutive name (2,2′-oxydiacetic acid and [(carboxymethyl)oxy]acetic acid), or between a substitutive name and a functional class name (bromomethane and methyl bromide), but not between a coordination or binary name and an organic name, for example, when the choice could be between a substitutive name and coordination name (tetrachlorosilane and tetrachloridosilicon).

The nomenclature of organic compounds is considered as the set of different types of nomenclature based on the various operations described in P-13. The term nomenclature is usually associated with more than one kind of operation. **Substitutive nomenclature** may be regarded as based on substitutive, additive, and subtractive operations. **Functional class nomenclature** is essentially based on additive operations, but includes substituent group names formed by substitutive nomenclature. **Multiplicative nomenclature** is a subset of substitutive nomenclature based on cyclic parent hydrides, functionalized or not, functionalized acyclic parent hydrides, and heteroacyclic parent hydrides. **Skeletal replacement nomenclature** usually refers to replacement by ‘a’ terms and is thus often called just **‘a’ nomenclature**. Similarly, **conjunctive nomenclature,** is restricted to conjunction operations involving rings or ring systems substituted by a chain bearing a principal group named substitutively or having a retained name. Finally, **functional replacement nomenclature** defines the rules for the use of prefixes and infixes to indicate replacement of oxygen atoms or oxygen groups by nitrogen atoms, nitrogen groups, chalcogen atoms, halogen atoms, peroxy groups, etc. (see P-15.5).

Thus, the term nomenclature is not normally associated with only a single type of operation, and name formation within a nomenclature system consists of a series of operations of various types, for example the subtractive operation in the formation of double bonds and the functional replacement operation in the replacement of oxygen atoms by chalcogen or nitrogen atoms.

The term nomenclature also applies to families or classes of compounds, for instance **Nomenclature of Radicals and Ions, Phane Nomenclature** for naming compounds composed of chains and/or ring systems, and **Fullerene Nomenclature** to describe all operations necessary to name polycyclic carbon cage compounds and their derivatives. This term is also used to describe families of compounds of natural origin, for example, **Nomenclature of Natural Products** is based on the concept of stereoparents. The nomenclature of carbohydrates, of α-amino acids, peptides, lipids, and of some other compounds of biochemical significance is generally considered to be **Biochemical Nomenclature** and, as such, is published comprehensively separately.

P-15.1 SUBSTITUTIVE NOMENCLATURE

Substitutive nomenclature is based on the selection of a parent structure having substitutable hydrogen atoms (see P-15.1.5) which are substituted by nomenclaturally significant structural fragments represented either by prefixes and/or suffixes or only by prefixes. In substitutive nomenclature there are three kinds of parent structures, parent hydrides, functionalized parent hydrides, and functional parent compounds.

P-15.1.1 Parent hydrides

Parent hydrides are unbranched acyclic, cyclic structures, or acyclic/cyclic structures to which only hydrogen atoms are attached. They may have retained names as described in Chapters P-2 and P-3, semisystematic names for natural products (see P-101), or names derived by the systematic methods described in Chapters P-2 and P-3.

Examples

methane (PIN; retained name, P-21.1.1.1)

cyclohexane (PIN; P-22.1.1)

styrene (retained name, P-31.1.3.4); ethenylbenzene (PIN)

pyridine (retained name, PIN; P-22.2.1)

cholestane (retained name, Table 10.1, b)

Parent hydrides may be substituted by prefixes and/or suffixes. A complete substitutive name may be described schematically in Fig. 1.1.

Prefixes			**Parent**	**Endings**	**Suffixes**	
Detachable substitutive prefixes	Detachable saturation/ unsaturation prefixes	Nondetachable structure defining prefixes	Name of parent hydride	Unsaturation endings (ane/ene/ yne)	Functional suffixes	Cumulative suffixes

	(hydro/dehydro)					

Fig. 1.1 Order of components in substitutive names based on parent hydrides

P-15.1.2 Functional parent compounds

P-15.1.2.1 Functional parent compounds used in systematic organic nomenclature are structures having retained names that imply the presence of at least one characteristic group and which have one or more hydrogen atoms attached to at least one of its skeletal atoms or in which at least one of its characteristic groups can form at least one kind of functional modification. The modification of these functional parent compounds is limited as only detachable prefixes and cumulative suffixes can be added. Furthermore, preferred IUPAC functional parent compound names cannot be modified by changing the degree of hydrogenation by means of the prefixes hydro/dehydro, by changing the ending 'ane' into 'ene' or 'yne', or by modifing the structure by nondetachable prefixes, such as 'cyclo'.

Examples:

acetic acid (PIN; P-65.1.1)

aniline (PIN; P-62.2.1.1.1)

phosphonic acid (preselected name; P-67.1.1)

P-15.1.2.2 A second group of functional parent compounds is extensively used in the nomenclature of natural products, for which nondetachable prefixes, such as 'cyclo', 'nor', 'homo'; hydro/dehydro prefixes; and the endings 'ene', 'yne', etc., as specified in Chapter P-10.

Examples:

D-glucose (Table 10.2)

alanine (Table 10.4)

A complete preferred IUPAC substitutive name based on a functional parent compound may be described schematically as shown in Fig. 1.2.

Detachable substitutive prefixes	Name of functional parent compound	Cumulative suffixes

Fig. 1.2 Order of components in a substitutive name based on a functional parent compound

P-15.1.2.3 A functionalized parent hydride is a parent hydride substituted by a characteristic group suffix, for example, ethanamine (see P-62.2.1.2) and cyclohexanol (see P-63.1.2), and should not be confused with a functional parent compound.

P-15.1.3 Suffixes (see also P-33)

There are, in general, two kinds of suffixes, functional suffixes and cumulative suffixes.

(1) Functional suffixes are generally simple suffixes used for describing characteristic groups that express classes. For example, the classes ketones, acids, amines, and esters are denoted by the suffixes -one, -carboxylic acid, -amine, and -carboxylate, respectively. Functional suffixes are exclusive suffixes, as the presence of one suffix denoting the principal characteristic group excludes all other suffixes describing other characteristic groups that must be designated as prefixes.

(2) Cumulative suffixes are used to designate radicals, ions, radical ions, and related species, for example, -yl, -ium, -ide, as well as substituent groups. Cumulative suffixes are not exclusive. They can be combined with each other as well as with functional suffixes, for example, -aminyl, -nitrilium, -sulfaniumyl.

Examples:

$$CH_4 \longrightarrow CH_4^{\bullet+}$$

methane (PIN) → methaniumyl (PIN)
(parent hydride) → ('iumyl' is a cumulative suffix)

$$CH_3\text{-}CH_3 \longrightarrow CH_3\text{-}CH_2\text{-}NH_2 \longrightarrow CH_3\text{-}CH_2\text{-}NH_3^+$$

ethane (PIN)
(parent hydride)

ethanamine (PIN)
('amine' is a functional suffix)

ethanaminium (PIN)
('ium' is a cumulative suffix)

P-15.1.4 Position of the endings 'ane', 'ene', and 'yne'

The modification of the ending 'ane' to 'ene' or 'yne' in acyclic, cyclic and polycyclic parent hydrides is used to describe the subtractive operation that inserts double and triple bonds into saturated parent hydrides. These endings are cumulative and can be combined with functional suffixes.

P-15.1.5 Prefixes and their order in names

There are two kinds of prefixes, nondetachable and detachable. Nondetachable prefixes describe structural modifications to the parent structure creating new parent structures, for example, replacement prefixes, which can be either skeletal replacement ('a') prefixes (see P-15.4) or 'functional replacement prefixes' (see P-15.5). Detachable prefixes are of two types: prefixes that describe saturation or unsaturation ('hydro' and 'dehydro'); and prefixes that describe substitution, also called alphabetizable prefixes.

P-15.1.5.1 Nondetachable prefixes
P-15.1.5.2 Detachable hydro/dehydro prefixes
P-15.1.5.3 Detachable alphabetizable prefixes

Nondetachable prefixes, the detachable saturation prefixes ('hydro/dehydro'), and the detachable alphatizable prefixes are cited in names as indicated in Fig. 1.1 (see P-15.1.1).

P-15.1.5.1 Nondetachable prefixes

Nondetachable prefixes are permanently attached to the name of the parent structure in a given order, which normally matches the order of operations used to modify the parent structure. Prefixes describing the first operation are attached directly to the name of the parent structure; those resulting from a second operation are placed in front of those already introduced, and so on (this technique may be termed 'advancing backwards' from the name of the parent structure). The order is precisely prescribed for each category, as indicated below:

P-15.1.5.1.1 Nondetachable prefixes creating new parent structures:

(a) alicyclic rings and ring systems by prefixes such as: 'cyclo', 'bicyclo', 'tricyclo', etc.; 'spiro', 'dispiro', etc.;

(b) fused ring systems by fusion prefixes: 'benzo', 'naphtho', 'imidazo', etc.;

(c) bridged fused ring systems by the addition of bridge prefixes: 'methano', 'epoxy', etc.;

(d) spiro compounds formed by combining names of cyclic compounds in (a), (b), and/or (c).

P-15.1.5.1.2 Replacement of atoms other than hydrogen by other atoms.

This type of replacement, called 'skeletal replacement', is essentially the replacement of carbon atoms by heteroatoms; it takes place with acyclic and cyclic hydrocarbons generating new parent structures by using skeletal replacement ('a') prefixes, i.e., 'oxa', 'aza', 'thia', etc.

P-15.1.5.1.3 Indicated hydrogen (see P-14.7) is also a nondetachable prefix and is introduced in front of all other nondetachable prefixes.

P-15.1.5.2 Detachable hydro/dehydro prefixes

These two prefixes are introduced in names by an additive or subtractive operation; thus, they are not included in the category of detachable alphabetizable prefixes describing substitution (P-15.1.5.3). In names, they occupy a place between nondetachable prefixes and the detachable alphabetizable prefixes. These prefixes express modifications of the degree of hydrogenation of a ring or ring systen having the maximum number of noncumulative double bonds (a mancude structure) and are treated for numbering like the endings 'ene' and 'yne', which fulfill the same function. In names, the prefix 'dehydro' precedes the prefix 'hydro', when both are present. Simple numerical terms, such as 'di-', 'tri-', 'tetra-', etc., are used with 'hydro' and 'dehydro'.

P-15.1.5.3 Detachable alphabetizable prefixes

These prefixes describe substituent groups denoting characteristic groups that are not cited as principal characteristic group or groups derived from parent hydrides and are cited before the 'hydro-dehydro' prefixes, if present (see P-31.2), or nondetachable prefixes, if present, as indicated in Fig. 1.1. They are alphabetized in accordance with P-14.5.

P-15.1.6 Other components of substitutive names

In addition to the components described above, the following nomenclatural indicators are added, as required:

P-15.1.6.1 Multiplicative prefixes placed before suffixes and prefixes to indicate multiple occurrences.

P-15.1.6.2 Locants used to indicate positions of the parent structure at which modifications represented by suffixes, prefixes, and endings occur.

P-15.1.6.3 Stereodescriptors placed at the front of the complete name or name fragment to which they apply (see Chapter P-9).

P-15.1.7 Construction of substitutive names

This subsection describes the formation of substitutive names and the application of four general sets of rules dealing with numbering (P-14.4), locants (P-14.3), multiplicative prefixes (P-14.2), and alphanumerical order (P-14.5). These four sets of rules are applied in constructing names of most organic compounds. In the first set of examples, alkanes and branched alkanes are used. In the second set, the general rule of numbering is exemplified by saturated and unsaturated acyclic compounds denoted by suffixes. The full question of name construction is considered in P-45.

P-15.1.7.1 Naming of alkanes and branched alkanes

P-15.1.7.1.1 The names of alkanes are either the retained names, methane, ethane, propane, and butane; or are names formed systematically by adding the ending ‘ane’ to a basic multiplicative prefix, with elision of the final letter ‘a’ of the multiplicative term (See Chapter P-2).

Examples:

CH_4 methane (PIN)	$CH_3\text{-}CH_3$ ethane (PIN)	$CH_3\text{-}CH_2\text{-}CH_3$ propane (PIN)
$CH_3\text{-}CH_2\text{-}CH_2\text{-}CH_3$ butane (PIN)	$CH_3\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}CH_3$ pentane (PIN)	$CH_3\text{-}[CH_2]_8\text{-}CH_3$ decane (PIN)

P-15.1.7.1.2 Monovalent simple substituent groups derived from unbranched acyclic hydrocarbons (alkanes) by the removal of one hydrogen atom from a terminal carbon atom (subtractive operation) are named by replacing the ending ‘ane’ of the name of the hydrocarbon by ‘yl’ (see P-29.3.2.1) or, if one hydrogen atom is removed from a nonterminal carbon atom of a chain, by replacing the final ‘e’ of the name of the hydrocarbon by ‘yl’ (see P-29.3.2.2) (‘yl’ is a cumulative suffix, see Fig. 1.1, P-15.1.1).

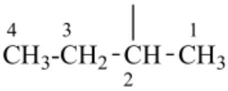
Examples:

$CH_3\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{–}$

butyl (preferred prefix)

$CH_3\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{–}$

pentyl (preferred prefix)

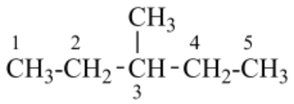


$$\overset{4}{CH_3}\text{-}\overset{3}{CH_2}\text{-}\underset{2}{\overset{|}{CH}}\text{-}\overset{1}{CH_3}$$

butan-2-yl (preferred prefix)

P-15.1.7.1.3 A saturated branched acyclic hydrocarbon is formed by substituting one or more substituent groups, formed as described in P-15.1.7.1.2, into the longest chain present in the structure (substitutive operation); it is named by prefixing the designations of the side chains, as formed in P-15.1.7.1.2, to the name of the longest chain [see P-15.1.7.1.4 for numbering].

Example:

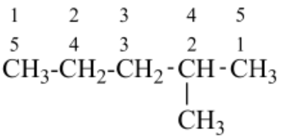


$$\overset{1}{CH_3}\text{-}\overset{2}{CH_2}\text{-}\underset{3}{\overset{\overset{CH_3}{|}}{CH}}\text{-}\overset{4}{CH_2}\text{-}\overset{5}{CH_3}$$

3-methylpentane (PIN)

P-15.1.7.1.4 The longest chain is numbered from one end to the other by arabic numbers, the direction being chosen so as to give the lower locants to the substituent groups (side chains) [see P-14.4 (f)]. The lower set of locants is defined as the set that, when compared term by term with other locant sets cited in order of increasing magnitude, has the lower term at the first point of difference (see P-14.3.5). The locants are placed immediately in front of the part of the name to which they refer. Identical simple substituent groups are indicated by multiplicative prefixes, such as ‘di’, ‘tri’, etc. [P-16.3.3 (b)]. For compound or complex substituent groups (see P-29.4 and P-29.5), the multiplicative prefixes ‘bis’, ‘tris’, ‘tetrakis-’, etc. (P-14.2.2) are used as described in P-16.3.5 (a).

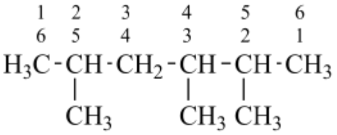
Examples:



$$\overset{\overset{1}{5}}{CH_3}\text{-}\overset{\overset{2}{4}}{CH_2}\text{-}\overset{\overset{3}{3}}{CH_2}\text{-}\underset{\underset{CH_3}{|}}{\overset{\overset{4}{2}}{CH}}\text{-}\overset{\overset{5}{1}}{CH_3}$$

incorrect numbering
correct numbering

2-methylpentane (PIN)



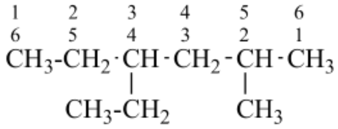
$$\begin{array}{cccccc} 1 & 2 & 3 & 4 & 5 & 6 \\ 6 & 5 & 4 & 3 & 2 & 1 \\ \mathrm{H_3C\text{-}} & \mathrm{CH\text{-}} & \mathrm{CH_2\text{-}} & \mathrm{CH\text{-}} & \mathrm{CH\text{-}} & \mathrm{CH_3} \\ & | & & | & | & \\ & \mathrm{CH_3} & & \mathrm{CH_3} & \mathrm{CH_3} & \end{array}$$

incorrect numbering
correct numbering

2,3,5-trimethylhexane (PIN)
(not 2,4,5-trimethylhexane;
the locant set 2,3,5 is lower than 2,4,5)

P-15.1.7.1.5 If two or more different substituent groups are present, they are cited in names in alphanumerical order (see P-14.5). When two or more substituent groups occupy equivalent positions, the one to be assigned the lower locant is that one cited first in the name.

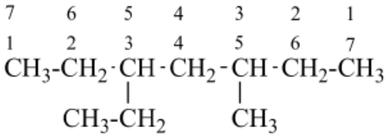
Examples:



$$\begin{array}{cccccc} 1 & 2 & 3 & 4 & 5 & 6 \\ 6 & 5 & 4 & 3 & 2 & 1 \\ \mathrm{CH_3\text{-}} & \mathrm{CH_2\text{-}} & \mathrm{CH\text{-}} & \mathrm{CH_2\text{-}} & \mathrm{CH\text{-}} & \mathrm{CH_3} \\ & & | & & | & \\ & & \mathrm{CH_3\text{-}CH_2} & & \mathrm{CH_3} & \end{array}$$

incorrect numbering
correct numbering

4-ethyl-2-methylhexane (PIN)
(not 3-ethyl-5-methylhexane;
the locant set 2,4 is lower than 3,5)



$$\begin{array}{ccccccc} 7 & 6 & 5 & 4 & 3 & 2 & 1 \\ 1 & 2 & 3 & 4 & 5 & 6 & 7 \\ \mathrm{CH_3\text{-}} & \mathrm{CH_2\text{-}} & \mathrm{CH\text{-}} & \mathrm{CH_2\text{-}} & \mathrm{CH\text{-}} & \mathrm{CH_2\text{-}} & \mathrm{CH_3} \\ & & | & & | & & \\ & & \mathrm{CH_3\text{-}CH_2} & & \mathrm{CH_3} & & \end{array}$$

incorrect numbering
correct numbering

3-ethyl-5-methylheptane (PIN)
(not 5-ethyl-3-methylheptane;
the lower locant must be assigned to the
substituent group that is cited first)

P-15.1.7.2 The numbering rules

The following examples illustrate the rule for numbering described in P-14.4. This rule establishes an order of priority among different nomenclatural features for assignment of the lowest possible locants.

P-15.1.7.2.1 Alcohols are named by attaching the suffix ‘ol’ to the name of the parent hydride, with elision of the final letter ‘e’ in the parent hydride, if present. When alone in the structure, the characteristic group(s) must receive the lowest locant(s) possible, which is (are) cited immediately in front of the suffix (see P-14.3.2).

Example:

$$\overset{3}{\mathrm{CH_3}}\text{-}\overset{2}{\mathrm{CH_2}}\text{-}\overset{1}{\mathrm{CH_2}}\text{-}\mathrm{OH}$$

propan-1-ol (PIN)

P-15.1.7.2.2 Alkenes are acyclic branched or unbranched hydrocarbons having one double bond. When one double bond is present, an unbranched alkene is named by changing the ending ‘ane’ in the name of the alkane having the same number of carbon atoms to the ending ‘ene’ (see P-31.1). The double bond is assigned the lowest locant possible, which is placed immediately in front of the ending ‘ene’ (see P-14.3.2)

Example:

$$\overset{1}{\mathrm{CH_2}}{=}\overset{2}{\mathrm{CH}}\text{-}\overset{3}{\mathrm{CH_2}}\text{-}\overset{4}{\mathrm{CH_3}}$$

but-1-ene (PIN)

P-15.1.7.2.3 When several nomenclatural features are present in a structure, lowest locants are assigned in accordance with P-14.4. For example, in an unsaturated alcohol having one substituent group, lowest locants are assigned in the order:

(a) characteristic group cited as suffix (-ol);

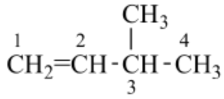
(b) unsaturation (‘ene‘ ending, for example);

(c) detachable alphabetized prefixes (a methyl group, for instance);.

The following examples illustrate the application of this rule

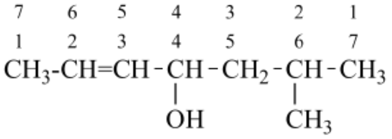
$$\overset{4}{C}H_2=\overset{3}{C}H\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}H_2\text{-}OH$$

but-3-en-1-ol (PIN)



$$\overset{1}{C}H_2=\overset{2}{C}H\text{-}\underset{3}{\overset{\overset{CH_3}{|}}{C}H}\text{-}\overset{4}{C}H_3$$

3-methylbut-1-ene (PIN)



$$\begin{array}{ccccccc} 7 & 6 & 5 & 4 & 3 & 2 & 1 \\ 1 & 2 & 3 & 4 & 5 & 6 & 7 \\ CH_3\text{-} & CH= & CH\text{-} & CH\text{-} & CH_2\text{-} & CH\text{-} & CH_3 \\ & & & | & & | & \\ & & & OH & & CH_3 & \end{array}$$

incorrect numbering
correct numbering

6-methylhept-2-en-4-ol (PIN)
(not 2-methylhept-5-en-4-ol)

P-15.1.8 Substitution rules for parent structures with retained names

The following rules describe the substitutability of parent structures having retained names found in P-22.1.2, P-22.1.3, Tables 2.2, 2.3, 2.7, 2.8, Tables 3.1, 3.2, and for functional parent compounds given in P-34. These rules do not apply to functional parent compounds used in the nomenclature of natural products (see Chapter P-10), where specific rules apply.

P-15.1.8.1 Type 1 Unlimited substitution by substituent groups cited either as suffixes or prefixes; this applies mainly to parent hydrides
P-15.1.8.2 Type 2 Limited substitution generalized as follows:
  Type 2a Substitution limited to substituent groups cited as prefixes in accordance with the seniority of functional groups explicitly expressed or implied in the functional parent compound name;
  Type 2b Substitution limited to substituent groups that are compulsory prefixes (see Table 5.1);
  Type 2c Substitution for parent structures not covered by Types 2a or 2b.
P-15.1.8.3 Type 3 Substitution of any kind is not allowed

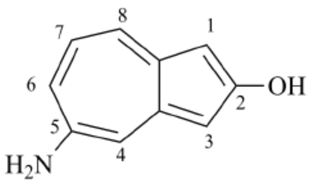
P-15.1.8.1 Substitution rules for Type 1 retained names

Type 1 retained names of parent hydrides described in Chapters P-2 and P-3 have unlimited substitution by substituent groups cited either as suffixes or prefixes.

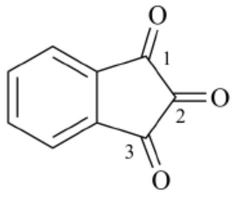
Examples:

$$HOO\overset{1}{C}\text{-}\overset{2}{C}HF\text{-}\overset{3}{C}H(NO_2)\text{-}\overset{4}{C}OOH$$

2-fluoro-3-nitrobutanedioic acid (PIN)
(butane is a retained name)



5-aminoazulen-2-ol (PIN; azulene is a retained name)
(not 2-hydroxyazulen-5-amine)



indane-1,2,3-trione
1*H*-indene-1,2,3-trione (PIN)

P-15.1.8.2 Substitution rules for Type 2 retained names

Substitution of parent hydrides with retained names and of functional parent compounds whose retained names explicitly or implicitly express the presence of a characteristic group normally expressed as a suffix, such as '-one', or a functional class, such as 'ether', is limited in different ways as described in the following subsections. Rules for the substitution of inorganic oxo acids used as functional parents and parent structures are described in P-67.

P-15.1.8.2.1 Substitution rules for Type 2a retained names

Type 2a retained names include functional parent compounds whose name expresses or implies a characteristic group expressed as suffix in systematic names.

P-15.1.8.2.1.1 Substitution by substituent groups, expressed as prefixes, having a lower seniority than that denoted by the suffix is allowed.

Examples:

$H_2N-CH_2-CO-CH_3$

aminoacetone

1-aminopropan-2-one (PIN)

$HS-CH_2-COOH$

sulfanylacetic acid (PIN)

A suffix explicitly or implicitly present cannot be expressed as a prefix;

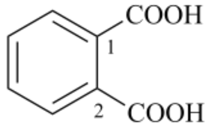
Examples:

$HOOC-CH_2-COOH$

propanedioic acid (PIN)

malonic acid

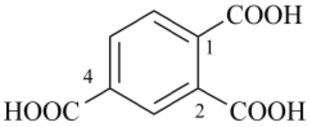
(not 2-carboxyacetic acid)



benzene-1,2-dicarboxylic acid (PIN)

phthalic acid

(not 2-carboxybenzoic acid)



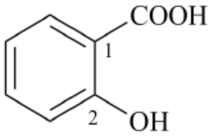
benzene-1,2,4-tricarboxylic acid (PIN)

(not 2,4-dicarboxybenzoic acid;

not 4-carboxyphthalic acid)

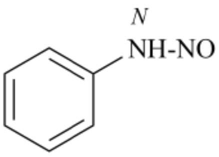
P-15.1.8.2.1.2 The senior characteristic group or functional class name must be expressed in the name.

Examples:



2-hydroxybenzoic acid (PIN)

(not 2-carboxyphenol)



phenylnitrous amide (PIN)

N-nitrosoaniline

P-15.1.8.2.2 Substitution rules for Type 2b retained names

Type 2b retained names include parent compounds explicitly or implicitly devoid of suffixes; acetylene (PIN) and allene are examples. Substitution of these parent compounds is possible by using specifically designated prefixes only.

The following characteristic groups cited can be used to substitute parent structures of Type 2b (ring and the side chain if required): halides –Br, –Cl, –F, –I, pseudohalides $-N_3$, –NCO (and chalcogen analogues), –NC, substituent groups derived from the halogen oxo acids –ClO, $-ClO_2$, $-ClO_3$ (similarly for groups in which Cl is replaced by Br or I), $-NO_2$ and –NO, and –OR (R = alkyl groups), and chalcogen analogues, and –SO-R and $-SO_2$-R, and Se and Te analogues (see Table 5.1).

Examples:

$\mathrm{Br{-}C{\equiv}C{-}H}$
bromoacetylene
bromoethyne (PIN)

$\mathrm{Cl{-}\overset{1}{C}H{=}\overset{2}{C}{=}\overset{3}{C}H{-}Cl}$
1,3-dichloroallene
1,3-dichloropropa-1,2-diene (PIN)

P-15.1.8.2.3 Substitution rules for Type 2c retained names

Type 2c retained names are functional parent compounds that are not included in Type 2b, for example, hydroxylamine (see P-68.3.1.1.1), formic acid (see P-65.1.8), and anisole (see P-34.1.1.4).

Examples:

$\mathrm{H_2N{-}O{-}CH_3}$
O-methylhydroxylamine (PIN)
[not methoxyamine (see P-68.3.1.1.1.2)]

HS-CO-OH
carbonothioic S-acid (PIN)
[not sulfanylformic acid (see P-65.1.8.1)]

P-15.1.8.3 Substitution rules for Type 3 retained names

No substitution of any kind is allowed for retained names of parent hydrides and functional parent compounds of type 3. However, functionalization of characteristic groups, such as the formation of esters, anhydrides, and salts is allowed

Examples:

$\mathrm{Cl{-}CH_2{-}CH_2{-}COOH}$
3-chloropropanoic acid (PIN)
(not 3-chloropropionic acid)

$\mathrm{CH_3{-}CH_2{-}CO{-}O{-}CH_2{-}CH_3}$
ethyl propanoate (PIN)
ethyl propionate

P-15.2 FUNCTIONAL CLASS NOMENCLATURE

P-15.2.0 Introduction

Functional class nomenclature was quite important in the early days of organic chemistry when many compounds were named using class names. The procedures were identical with those of substitutive nomenclature except that suffixes were never used. Substituent groups, called ‘radicals’ in early nomenclature, were used in association with a name denoting the class; this nomenclature was called ‘radicofunctional nomenclature’. With time, substitutive nomenclature replaced functional class nomenclature in all but a few instances. In the context of IUPAC preferred names, substitutive nomenclature is the primary way for naming organic compounds; functional class nomenclature is reduced to a strict minimum.

The notion of functional class nomenclature is also applied to compounds that are named using a class name, but not necessarily preceded by a substituent group name. To that purpose, ‘functional modifiers’ are used to indicate a functional change, for example the change of acid to anhydride, as in acetic anhydride, or the formation of derivatives of ketones, for example, butan-2-one oxime.

It is convenient to classify the main operation involved in functional class nomenclature as an additive one, as is done in P-13.3.3.2. However it is also possible (and probably more relevant from a historical point of view) to regard the process as one of specifying the substituent groups (‘radicals’) present in compounds for which a class name is given. For instance, the name ‘methyl alcohol’ (for CH_3-OH) consists of the name ‘methyl’ for the substituent group CH_3– and the class name ‘alcohol’ (for R-OH).

Functional class nomenclature is discussed in relation to the traditional use of substituent group names and the use of functional modifiers. Some names are formed on the basis of a class name, but are not considered as belonging to the functional class nomenclature. They are called ‘descriptive’ names, for example, ‘propanoic acid methyl ester’, and are never considered as IUPAC preferred names. The order of seniority of classes (see P-41) is given in the context of preferred IUPAC names.

P-15.2.1 Functional class nomenclature using substituent group names
P-15.2.2 Functional class nomenclature using functional modifiers
P-15.2.3 Seniority of functional classes
P-15.2.4 Polyfunctional compounds

P-15.2.1 Functional class nomenclature using substituent group names

P-15.2.1.1 Functional class names are formed by expressing the functional class name of the compound as one word and the remainder of the molecule as a monovalent group name cited as a separate word, placed in front of the class name. Preferred IUPAC functional class names are restricted to esters (P-65.6.3.2), acyl halides (P-65.5.1), and pseudohalides (see P-65.5.2). Alkyl glycosides receive also functional class names that are classified as approved names in carbohydrate nomenclature (see P-102.5.6.2).

Examples:

CH_3-CH_2-CO-O-CH_3
methyl propanoate (PIN)

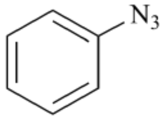
CH_3-CO-Cl
acetyl chloride (PIN)

C_6H_5-CO-CN
benzoyl cyanide (PIN)

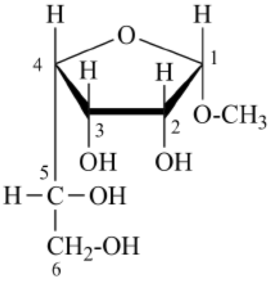
C_6H_5-CH_2-NCS
benzyl isothiocyanate
(isothiocyanatomethyl)benzene (PIN)

C_6H_5-NC
phenyl isocyanide
isocyanobenzene (PIN)

CH_3-OH
methyl alcohol
methanol (PIN)



phenyl azide
azidobenzene (PIN)



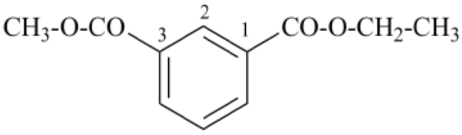
methyl α-D-gulofuranoside

P-15.2.1.2 When the functional class name refers to a characteristic group that is divalent, the two substituent groups attached to it are both expressed. When they are the same, appropriate numerical prefixes are used. When different, they are written as separate words, in alphanumerical order, locants being added as needed.

Examples:

CH_3-O-CO-CH_2-CH_2-CO-O-CH_3
dimethyl butanedioate (PIN)
dimethyl succinate

CH_3-CO-O-CH_2-CH_2-O-CO-CH_3
ethane-1,2-diyl diacetate (PIN)
ethylene diacetate



ethyl methyl benzene-1,3-dicarboxylate (PIN)

CH_3-CH_2-CO-CH_2-CH_3
diethyl ketone
pentan-3-one (PIN)

CH_3-CH_2-CO-CH_3
ethyl methyl ketone
(not methyl ethyl ketone)
butan-2-one (PIN)

P-15.2.2 Functional class nomenclature using functional modifiers

Many derivatives of principal characteristic groups or functional parent compounds (see P-34) may be named by modifiers consisting of one or more separate words placed after the name of the parent structure. This method is most useful in an indexing environment, but it is the only method used for naming acyclic anhydrides (see P-65.7.1), *N*-oxides, *N*-sulfides, *N*-selenides, and *N*-tellurides (see P-62.5) in the context of preferred IUPAC names.

Examples:

CH_3-CO-O-CO-CH_3
acetic anhydride (PIN)
(the term 'acid' is replaced by 'anhydride')

$(CH_3)_3NO$
N,*N*-dimethylmethanamine *N*-oxide (PIN)
trimethylazane *N*-oxide
trimethylamine *N*-oxide
(traditional name, but cannot be substituted)

Functional modifiers are still acceptable for general nomenclature purposes, but the preferred IUPAC names are substitutive names for azines, oximes, hydrazones, semicarbazones, carbohydrazones, acetals, and hemiacetals.

Examples:

CH_3-CH_2-CH=N-OH
propanal oxime
(the term 'oxime' is added to the name of the carbonyl compound)
N-propylidenehydroxylamine
N-hydroxypropan-1-imine (PIN)

CH_3-CH_2-CH=N-NH_2
propanal hydrazone
propylidenehydrazine (PIN)

$(CH_3)_2C$=N-NH-CO-NH_2
acetone semicarbazone
2-(propan-2-ylidene)hydrazine-1-carboxamide (PIN)

CH_3-CH_2-CH(O-CH_3)$_2$
propanal dimethyl acetal
1,1-dimethoxypropane (PIN)

CH_3-CH_2-CH_2-CO-OCH_3
butanoic acid methyl ester
methyl butanoate (PIN)

P-15.2.3 Seniority of functional classes.

When two classes are present and both named by functional class nomenclature, the senior class must be chosen in accordance with the seniority order of classes (see P-41). The relevant order for preferred IUPAC names is anhydrides, esters, acyl halides. The seniority order of halides and pseudohalides is discussed in P-65.5. The senior class is expressed by functional class nomenclature and the lower ranking classes are expressed by prefixes, as usual, in that part of the name that is constructed by substitutive nomenclature.

Examples:

$Cl\text{-}\overset{4}{C}O\text{-}CH_2\text{-}CH_2\text{-}\overset{1}{C}O\text{-}O\text{-}CH_3$
methyl 4-chloro-4-oxobutanoate (PIN)
methyl 3-(chlorocarbonyl)propanoate
methyl 3-carbonochloridoylpropanoate

$Cl\text{-}CH_2\text{-}OH$
chloromethyl alcohol
chloromethanol (PIN)
(an alcohol is senior to a halide)

$NC\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}O\text{-}Cl$
cyanoacetyl chloride (PIN)
(an acyl chloride senior to a nitrile)

$CH_3O\text{-}\overset{4}{C}H_2\text{-}CH_2\text{-}\overset{1}{C}O\text{-}OCH_3$
methyl 4-methoxybutanoate (PIN)
(an ester senior to an ether)

P-15.2.4 Polyfunctional compounds

Functional class names for polyfunctional compounds are not recommended. Substitutive nomenclature is preferred.

$HO\text{-}CH_2\text{-}CH_2\text{-}CO\text{-}CH_3$
4-hydroxybutan-2-one (PIN; substitutive name)
2-hydroxyethyl methyl ketone (functional class name)

P-15.3 MULTIPLICATIVE NOMENCLATURE

- P-15.3.0 Introduction
- P-15.3.1 General methodology
- P-15.3.2 Construction of multiplicative names
- P-15.3.3 Identical structural units linked by unsymmetrical multiplicative groups
- P-15.3.4 Limitations of multiplicative nomenclature

P-15.3.0 Introduction

Multiplicative nomenclature is used to name assemblies of identical parent structures. There are two subsets of multiplicative nomenclature:

(1) A subset of substitutive nomenclature in which the identical structural units are linked by di- or polyvalent substituent groups (see P-15.3.1);

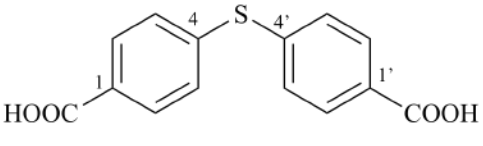
(2) A subset of functional class nomenclature in which the identical structural units are linked by a di- or polyvalent nonacidic residue (this subset is only used to name esters, for which see P-65.6.3.2, and leads to names such as 'ethane-1,2-diyl diacetate' for $CH_3COO\text{-}CH_2\text{-}CH_2\text{-}OCOCH_3$).

In the subset of multiplicative nomenclature as a subset of substitutive nomenclature, two or more identical units, for example, parent structures, linked by di- or polyvalent substituent groups (called 'multiplicative atoms or groups' or 'linking atoms or groups') can be named in two ways:

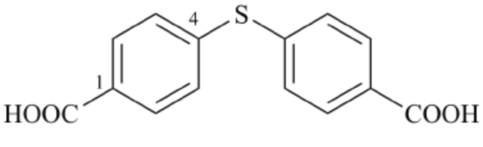
(a) by multiplicative nomenclature, in which two or more parent structures are connected by symmetrical or unsymmetrical single or concatenated substituent groups; and

(b) by substitutive nomenclature (see P-15.1) in which one of the parent structures is chosen as the senior parent structure and the remainder of the structure is expressed by substituent prefixes.

For example, the following compound can be named 4,4′-sulfanediyldibenzoic acid (PIN) [numbering shown in (**I**)] using multiplicative nomenclature, a name that includes both of the benzoic acid groups in the name of the parent structure.



(**I**)



(**II**)

Alternatively, it can be named 4-[(4-carboxyphenyl)sulfanyl]benzoic acid by substitutive nomenclature [numbering shown in (**II**)], a name that includes only one of the benzoic acid groups in the name of the parent structure; the other benzoic acid group is expressed as a prefix.

In this section, the general principles for construction of multiplicative names are discussed. The rules for the use of multiplicative nomenclature in constructing preferred IUPAC names are given in P-51.3.

Multiplicative nomenclature is now extended to cyclic structures with or without characteristic groups; chains composed only of carbon atoms continue to be excluded. In past recommendations, multiplicative nomenclature was limited to compounds having characteristic groups expressed as suffixes or implied by a retained name, and for heterocyclic parent hydrides. The system now has also been expanded to allow substitution on the central unit of a multiplying group (P-15.3.1.2.1.2) and the use of nonsymmetrical central units under specific conditions (P-15.3.3.1).

P-15.3.1 General methodology

P-15.3.1.1 Identical parent structures
P-15.3.1.2 Multiplicative substituent groups
P-15.3.1.3 Multiplicative name formation

P-15.3.1.1 Identical structural units

There are four types of identical parent structures in multiplicative nomenclature:

(a) cyclic parent hydrides, mancude or saturated;

(b) mononuclear or polynuclear acyclic parent hydrides with the exception of saturated or unsaturated acyclic hydrocarbons;

(c) cyclic or acyclic parent hydrides substituted by characteristic groups expressed as suffixes, i.e., functionalized parent hydrides (see P-15.1.2.3);

(d) functional parent compounds having substitutable hydrogen atoms, for example, acetic acid or phosphonic acid (see P-15.1.2.1).

Identical parent structures must be attached to multiplicative substituent groups by identical bonds (single, double, or triple) and be identically substituted.

P-15.3.1.2 Multiplicative substituent groups

There are two types of multiplicative substituent groups:

P-15.3.1.2.1 Simple multiplicative atoms or groups
P-15.3.1.2.2 Concatenated multiplicative groups

P-15.3.1.2.1 Simple multiplicative atoms or groups

P-15.3.1.2.1.1 Any simple polyvalent substituent group (see P-29.1 for definition) may be used as a multiplicative substituent group when attached to two or more identical structural units.

$–CH_2–$
methylene (preferred prefix)
(not methanediyl)

–O–
oxy (preselected prefix)

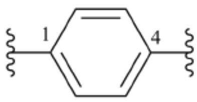
–S–
sulfanediyl (preselected prefix)
thio

–OO–
peroxy (preselected prefix)
(dioxy is no longer recommended)

–SS–
disulfanediyl (preselected prefix)
dithio

–N<
nitrilo (preselected prefix)

The prefix ‘nitrilo’, –N< ,is used as the preselected prefix only when the three bonds are attached to different atoms; it is no longer to be used for the structure –N=, which now is named as the preselected prefix ‘azanylylidene’.



1,4-phenylene (also 1,2- and 1,3-isomers;
preferred prefixes)

$-OC-CH_2-CH_2-CO-$
butanedioyl (preferred prefix)
succinyl

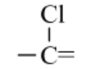
$>\overset{1}{C}H-\overset{2}{C}H_2-$
ethane-1,1,2-triyl (preferred prefix)

$-\overset{1}{C}H=\overset{2}{C}H-\overset{3}{C}H_2-$
prop-1-ene-1,3-diyl (preferred prefix)

P-15.3.1.2.1.2 Substitution, expressed by prefixes or implied, is allowed on simple multiplicative groups, symmetrical or unsymmetrical, generating substitutive compound or complex (see P-29.1 for definitions) multiplicative groups.

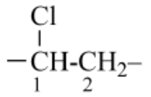
Examples:

$ClCH<$
chloromethylene (preferred prefix;
a compound multiplicative group)



$-\overset{Cl}{\overset{|}{C}}=$

chloromethanylylidene (preferred prefix;
a compound multiplicative group)



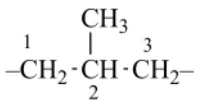
$-\underset{1}{\overset{Cl}{\overset{|}{C}H}}-\underset{2}{C}H_2-$

1-chloroethane-1,2-diyl (preferred prefix;
a compound multiplicative group)

$CH_3-N<$
methylazanediyl (preferred prefix;
a compound multiplicative group)
(no longer methylimino)

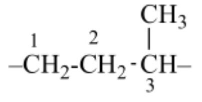
> The name azanediyl (preselected prefix) derived from the preselected parent hydride name ‘azane’ is recommended for the multiplicative substituent group –NH– ; the name imino (also a preselected prefix) is used only for =NH as a substituent.

$ClCH_2-P<$
(chloromethyl)phosphanediyl (preferred prefix;
a complex multiplicative group)



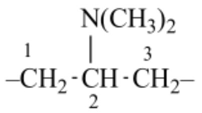
$-\overset{1}{C}H_2-\underset{2}{\overset{CH_3}{\overset{|}{C}H}}-\overset{3}{C}H_2-$

2-methylpropane-1,3-diyl (preferred prefix)



$-\overset{1}{C}H_2-\overset{2}{C}H_2-\underset{3}{\overset{CH_3}{\overset{|}{C}H}}-$

butane-1,3-diyl (preferred prefix; see P-29.3.2.2)
1-methylpropane-1,3-diyl (see P-29.4.1)



$-\overset{1}{C}H_2-\underset{2}{\overset{N(CH_3)_2}{\overset{|}{C}H}}-\overset{3}{C}H_2-$

2-(dimethylamino)propane-1,3-diyl (preferred prefix)

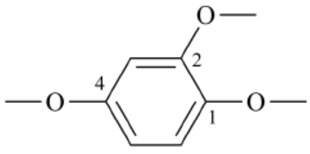
P-15.3.1.2.2 Concatenated multiplicative groups

P-15.3.1.2.2.1 Concatenation is the method used for the formation of multipart di- and polyvalent multiplicative substituent groups. A concatenated multiplicative group is formed by first citing the central multiplicative substituent group, followed by a multiplicative prefix, such as 'di', 'tri', etc. or 'bis', 'tris', etc., and then, in order, and in the direction toward the identical parent structures, the names of successive di- or polyvalent substituent groups.

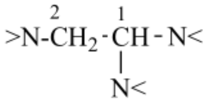
Examples:

$–O-CH_2-O–$
methylenebis(oxy)
(preferred prefix)
(not methylenedioxy; dioxy could be ambiguous,
because it could be 'peroxy' or twice 'oxy' [see P-15.3.1.2.1.1, P-16.3.6 (b).]

$–CH_2-O-CH_2–$
oxybis(methylene) (preferred prefix)



benzene-1,2,4-triyltris(oxy) (preferred prefix)



$$\overset{2}{>N-CH_2}-\underset{N<}{\overset{1}{CH}}-N<$$

ethane-1,1,2-triyltrinitrilo (preferred prefix)

$–CH_2-NH-CO-CH_2-CO-NH-CH_2–$
propanedioylbis(azanediylmethylene) (preferred prefix)

Note: When two or more successive multiplicative groups follow the central multiplicative group they are not prefixed by separate multiplicative prefixes. Accordingly, the preferred IUPAC name for the example just above is NOT propanedioylbis(azanediyl)bis(methylene).

P-15.3.1.2.2.2 When polyvalent substituent groups of the 'yl/ylidene' type that have no locants and are cited in a prescribed order are used in a multipart multiplicative substituent group, concatenation occurs by adding a monovalent free valence of the 'yl' type to another monovalent free valence of the 'yl' type, and similarly for free valences of the 'ylidene' type.

Examples:

–CH=N-O-N=CH–
oxybis(azanylylidenemethanylylidene) (preferred prefix)
[not oxybis(nitrilomethanylylidene)]

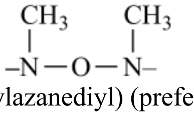
–O-N=CH-CH=N-O–
ethanediylidenebis(azanylylideneoxy) (preferred prefix)

–O-N=C=N-O–
methanediylidenebis(azanylylideneoxy) (preferred prefix)

=CH-N=C=N-CH=
methanediylidenebis(azanylylidenemethanylylidene) (preferred prefix)
[not methanediylidenebis(nitrilomethanylylidene)]

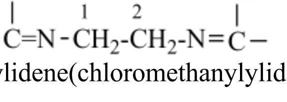
P-15.3.1.2.2.3 Substitution on the central substituent group and on successive substituent groups of a concatenated multiplicative substituent group is allowed provided that the sequence of atoms and bonds, starting at the central substituent group, are identical in each of the branches.

Examples:



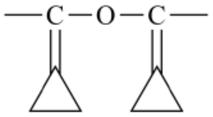
$$–\overset{CH_3}{N}-O-\overset{CH_3}{N}–$$

oxybis(methylazanediyl) (preferred prefix)



$$-\overset{Cl}{C}=N-\overset{1}{CH_2}-\overset{2}{CH_2}-N=\overset{Cl}{C}-$$

ethane-1,2-diylbis[azanylylidene(chloromethanylylidene)] (preferred prefix)

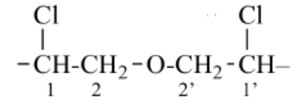


oxybis(cyclopropylidenemethylene) (preferred prefix)

Note: The preferred prefix given here would be ambiguous if the suffix 'ylidene' were not limited to the indication of double bonds (see P-29.2); it could refer to a structure in which the cyclopropane bonds went to the CH_2 group and the oxygen atom as single bonds; however, the latter structure would have the preferred IUPAC prefix oxybis(cyclopropane-1,1-diylmethylene)

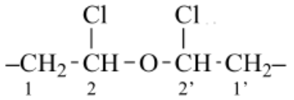
P-15.3.1.2.2.4 Numbering of the components of a multipart di- or trivalent multiplicative substituent group, when necessary, is achieved by attributing lowest locants to the atoms that are at the end of the component nearest to the multiplied parent structure, except where the component has a fixed numbering. The locants attached to the multiplied parent structure are cited last. When there is no choice the locants are cited in increasing numerical order.

Examples:



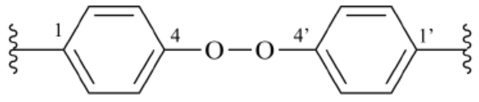
$$-\underset{1}{\overset{\overset{\mathrm{Cl}}{|}}{\mathrm{CH}}}-\underset{2}{\mathrm{CH_2}}-\mathrm{O}-\underset{2'}{\mathrm{CH_2}}-\underset{1'}{\overset{\overset{\mathrm{Cl}}{|}}{\mathrm{CH}}}-$$

oxybis(1-chloroethane-2,1-diyl) (preferred prefix)
oxybis(1-chloroethylene)

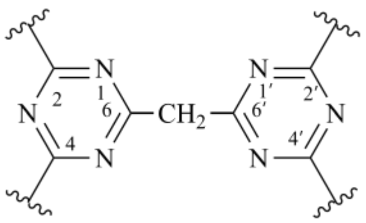


$$-\underset{1}{\mathrm{CH_2}}-\underset{2}{\overset{\overset{\mathrm{Cl}}{|}}{\mathrm{CH}}}-\mathrm{O}-\underset{2'}{\overset{\overset{\mathrm{Cl}}{|}}{\mathrm{CH}}}-\underset{1'}{\mathrm{CH_2}}-$$

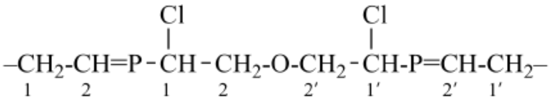
oxybis(2-chloroethane-2,1-diyl) (preferred prefix)
oxybis(2-chloroethylene)



peroxydi(4,1-phenylene) (preferred prefix)
[not dioxydi(4,1-phenylene)]

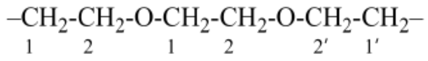


methylenedi(1,3,5-triazine-6,2,4-triyl) (preferred prefix)



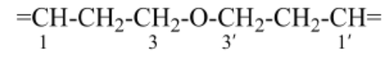
$$-\underset{1}{\mathrm{CH_2}}-\underset{2}{\mathrm{CH}}=\mathrm{P}-\underset{1}{\overset{\overset{\mathrm{Cl}}{|}}{\mathrm{CH}}}-\underset{2}{\mathrm{CH_2}}-\mathrm{O}-\underset{2'}{\mathrm{CH_2}}-\underset{1'}{\overset{\overset{\mathrm{Cl}}{|}}{\mathrm{CH}}}-\mathrm{P}=\underset{2'}{\mathrm{CH}}-\underset{1'}{\mathrm{CH_2}}-$$

oxybis[(1-chloroethane-2,1-diyl)phosphanylylideneethan-1-yl-2-ylidene]
(preferred prefix; the numbering of ethan-1-yl-2-ylidene is fixed)



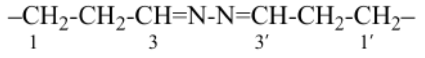
$$-\underset{1}{\mathrm{CH_2}}-\underset{2}{\mathrm{CH_2}}-\mathrm{O}-\underset{1}{\mathrm{CH_2}}-\underset{2}{\mathrm{CH_2}}-\mathrm{O}-\underset{2'}{\mathrm{CH_2}}-\underset{1'}{\mathrm{CH_2}}-$$

ethane-1,2-diylbis(oxyethane-2,1-diyl) (preferred prefix)



$$=\underset{1}{\mathrm{CH}}-\mathrm{CH_2}-\underset{3}{\mathrm{CH_2}}-\mathrm{O}-\underset{3'}{\mathrm{CH_2}}-\mathrm{CH_2}-\underset{1'}{\mathrm{CH}}=$$

oxydi(propan-1-yl-3-ylidene) (preferred prefix)



$$-\underset{1}{\mathrm{CH_2}}-\mathrm{CH_2}-\underset{3}{\mathrm{CH}}=\mathrm{N}-\mathrm{N}=\underset{3'}{\mathrm{CH}}-\mathrm{CH_2}-\underset{1'}{\mathrm{CH_2}}-$$

hydrazinediylidenedi(propan-1-yl-3-ylidene) (preferred prefix;
the numbering of propan-1-yl-3-ylidene is fixed)

P-15.3.1.3 Multiplicative name formation

Multiplicative names are formed in accordance with the number of occurrences of identical structural units as defined in P-15.3.1.1 and the relationship of the linking multiplicative substituent group to the identical structural units.

When a compound contains identical structural units as defined in P-15.3.1.1 linked by a symmetrical simple, compound, complex, or concatenated multiplicative group (a di- or polyvalent substituent group), it is named by stating successively:

(a) the locants for the positions of substitution of the linking multiplicative substituent atom or group to the identical parent structural unit (the locant 1 is omitted when alone in the name of a mononuclear parent hydride);

(b) the name of the linking multiplicative substituent atom or group;

(c) the numerical prefix ‘di’ , ‘tri’, etc.; and/or ‘bis-’, ‘tris-’, etc., with no elision of the final vowel before the name of the identical parent structural unit;

(d) the name of one of the identical structural units including the principal characteristic group and substituents, if any, enclosed in appropriate enclosing marks (see P-16.5).

The numbering of the identical parent structural unit is retained and, when there is a choice, the locants of the point of substitution by the linking multiplicative substituent groups on the identical parent structure are as low as possible.

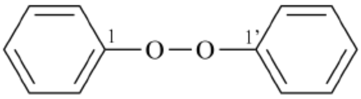
P-15.3.2 Construction of multiplicative names

P-15.3.2.1 Assemblies of identical structural units (see P-15.3.1.1)
P-15.3.2.2 Locants for nitrogen atoms in identical structural units
P-15.3.2.3 Use of multiplicative prefixes ‘bis’, ‘tris’, etc.
P-15.3.2.4 Substituted identical structural units (see P-15.3.1.1)

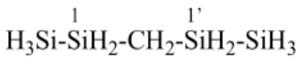
P-15.3.2.1 Assemblies of identical structural units (see P-15.3.1.1)

Retained and systematic names can be used as identical parent structural units. Primes, double primes, etc., are used to distinguish among the locants of the identical parent structural unit. When functionalized parent hydrides, i.e. parent structures substituted by groups expressed as suffixes (see P-15.1.2), have locants, they are enclosed in parentheses and preceded by a numerical prefix ‘di-’, ‘tri-’, etc. Unsubstituted functional parent compounds are preceded by the numerical prefix ‘di-’, ‘tri-, etc., but are not enclosed in parentheses, provided there is no ambiguity as described in P-15.3.2.3. Compound and complex multiplicative substituent groups are enclosed in parentheses, brackets or braces, as required (see P-16.5)

Examples:

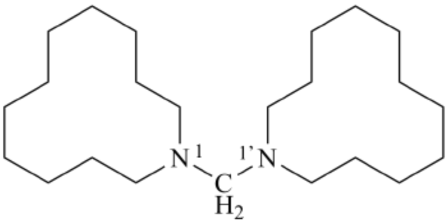


1,1′-peroxydibenzene (PIN)
(not dioxydibenzene)

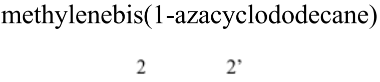


$H_3Si\text{-}\overset{1}{Si}H_2\text{-}CH_2\text{-}\overset{1'}{Si}H_2\text{-}SiH_3$

1,1′-methylenebis(disilane) (PIN)

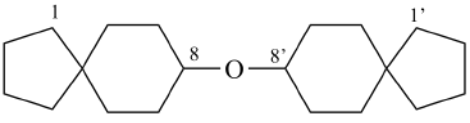


1,1′-methylenebis(1-azacyclododecane) (PIN)

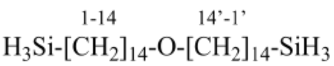


$HO\text{-}CH_2\text{-}\overset{2}{C}H_2\text{-}S\text{-}\overset{2'}{C}H_2\text{-}CH_2\text{-}OH$

2,2′-sulfanediyldi(ethan-1-ol) (PIN)
2,2′-thiodi(ethan-1-ol)

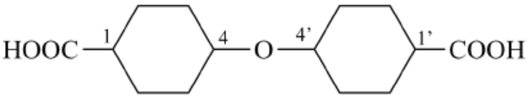


8,8′-oxydi(spiro[4.5]decane) (PIN)

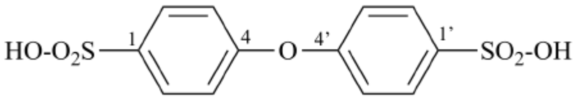


$H_3Si\text{-}\overset{1\text{-}14}{[CH_2]_{14}}\text{-}O\text{-}\overset{14'\text{-}1'}{[CH_2]_{14}}\text{-}SiH_3$

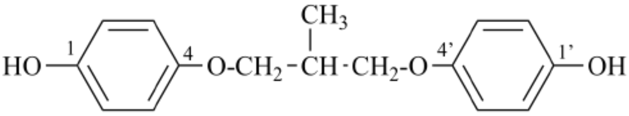
[oxydi(tetradecane-14,1-diyl)]bis(silane) (PIN)



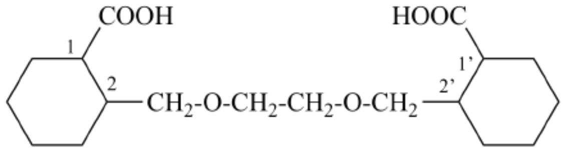
4,4′-oxydi(cyclohexane-1-carboxylic acid) (PIN)



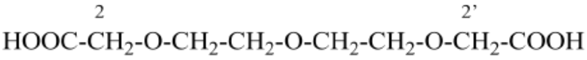
4,4′-oxydi(benzene-1-sulfonic acid) (PIN)



4,4′-[(2-methylpropane-1,3-diyl)bis(oxy)]diphenol (PIN)

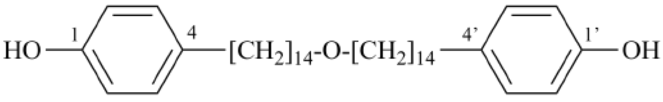


2,2′-[ethane-1,2-diylbis(oxymethylene)]di(cyclohexane-1-carboxylic acid) (PIN)

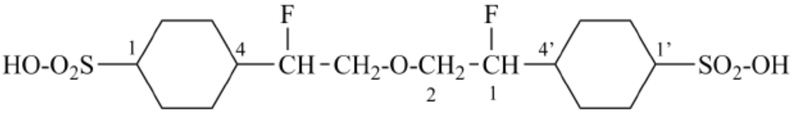


$\text{HOOC-}\overset{2}{\text{C}}\text{H}_2\text{-O-CH}_2\text{-CH}_2\text{-O-CH}_2\text{-CH}_2\text{-O-}\overset{2'}{\text{C}}\text{H}_2\text{-COOH}$

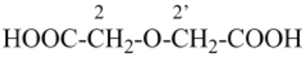
2,2′-[oxybis(ethane-2,1-diyloxy)]diacetic acid (PIN)



4,4′-[oxydi(tetradecane-14,1-diyl)]diphenol (PIN)

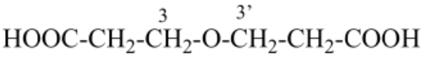


4,4′-[oxybis(1-fluoroethane-2,1-diyl)]di(cyclohexane-1-sulfonic acid) (PIN)



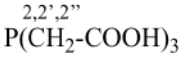
$\text{HOOC-}\overset{2}{\text{C}}\text{H}_2\text{-O-}\overset{2'}{\text{C}}\text{H}_2\text{-COOH}$

2,2′-oxydiacetic acid (PIN)



$\text{HOOC-CH}_2\text{-}\overset{3}{\text{C}}\text{H}_2\text{-O-}\overset{3'}{\text{C}}\text{H}_2\text{-CH}_2\text{-COOH}$

3,3′-oxydipropanoic acid (PIN)

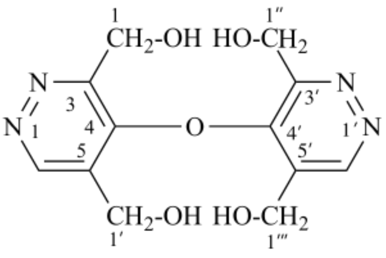


$\text{P(}\overset{2,2',2''}{\text{C}}\text{H}_2\text{-COOH)}_3$

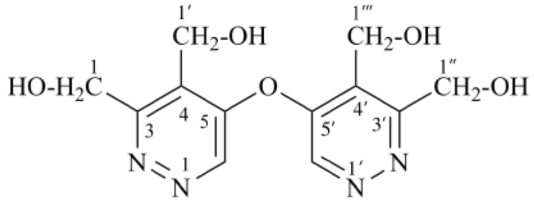
2,2′,2″-phosphanetriyltriacetic acid (PIN)

$\text{(HO)}_2\text{P(O)-CH}_2\text{-NH-CH}_2\text{-P(O)(OH)}_2$

[azanediylbis(methylene)]bis(phosphonic acid) (PIN)

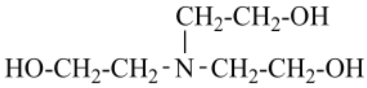


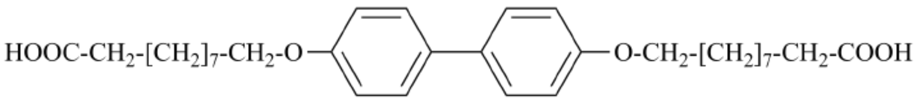
[oxydi(pyridazine-4,3,5-triyl)]tetramethanol (PIN)
(the locant set ‘3,4,5’ is lower than ‘4,5,6’ and the locant set ‘3,5’ is the lowest locant set of the pyridazine assigned to the junction to the multiplied parent structure)



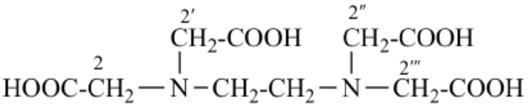
[oxydi(pyridazine-5,3,4-triyl)]tetramethanol (PIN)
(the locant set ‘3,4,5’ is lower than ‘4,5,6’;
the locant set ‘3,4’ is the lowest locant set of the pyridazine
assigned to the junction to the multiplied parent structure)

$H_2N\text{-}CH_2\text{-}CH_2\text{-}O\text{-}CH_2\text{-}CH_2\text{-}NH_2$
2,2′-oxydi(ethan-1-amine) (PIN)


$$\begin{array}{c} \qquad\qquad CH_2\text{-}CH_2\text{-}OH \\ \qquad | \\ HO\text{-}CH_2\text{-}CH_2\text{-}N\text{-}CH_2\text{-}CH_2\text{-}OH \end{array}$$
2,2′,2″-nitrilotri(ethan-1-ol) (PIN)

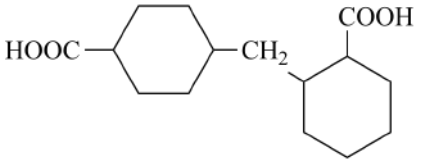


10,10′-[[1,1′-biphenyl]-4,4′-diylbis(oxy)]di(decanoic acid) (PIN).
[**Note:** A double set of square brackets appears in the above name because square brackets are required
for substituent names derived from ring assembly names (see P-16.5.2.1) and
brackets are needed to enclose the multiplicative substitutive name]

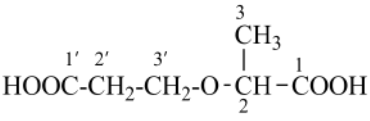

$$HOOC\text{-}\overset{2}{C}H_2\text{—}\overset{\overset{2'}{C}H_2\text{-}COOH}{\overset{|}{N}}\text{-}CH_2\text{-}CH_2\text{-}\overset{\overset{2''}{C}H_2\text{-}COOH}{\overset{|}{N}}\text{—}\overset{2'''}{C}H_2\text{-}COOH$$
2,2′,2″,2‴-(ethane-1,2-diyldinitrilo)tetraacetic acid
N,*N*′-(ethane-1,2-diyl)bis[*N*-(carboxymethyl)glycine]

P-15.3.2.1.1 If there is a choice, the greater number of primes is given to the locants of the parent structure having the higher numbered point of attachment to the multiplicative substituent group. Such names are not acceptable as preferred IUPAC names but may be used in general nomenclature; in these cases preferred IUPAC names are generated by substitutive nomenclature principles (see P-51.3.3).

Examples:



2,4′-methylenedi(cyclohexane-1-carboxylic acid) (multiplicative name)
2-[(4-carboxycyclohexyl)methyl]cyclohexane-1-carboxylic acid (PIN)
[not 4-[(2-carboxycyclohexyl)methyl]cyclohexane-1-carboxylic acid;
the substituent locant ‘2’ is lower than ‘4’ (see P-45.2.2)]

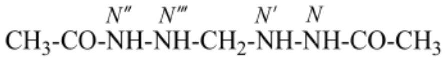

$$HOO\overset{1'}{C}\text{-}\overset{2'}{C}H_2\text{-}\overset{3'}{C}H_2\text{-}O\text{-}\underset{2}{\overset{\overset{3}{C}H_3}{\overset{|}{C}H}}\text{-}\overset{1}{C}OOH$$
2,3′-oxydipropanoic acid (multiplicative name)
2-(2-carboxyethoxy)propanoic acid (PIN)
[not 3-(1-carboxyethoxy)propanoic acid;
the substituent locant ‘2’ is lower than ‘3’ (see P-45.2.2)]

P-15.3.2.2 Locants for nitrogen atoms in identical parent structures

P-15.3.2.2.1 In multiplicative nomenclature, the use of primes on the italic letter *N* is used to differentiate among nitrogen atoms of identical structural units that contain one characteristic group with one or more nitrogen atoms.

Examples:

$$\overset{2}{C}H_3\text{-}\overset{1}{C}H_2\text{-}\overset{N}{N}H\text{-}CH_2\text{-}\overset{N'}{N}H\text{-}CH_2\text{-}CH_3$$
N,*N*′-methylenediethanamine

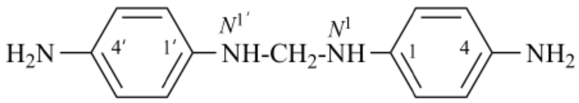


$CH_3\text{-}CO\text{-}\overset{N''}{NH}\text{-}\overset{N'''}{NH}\text{-}CH_2\text{-}\overset{N'}{NH}\text{-}\overset{N}{NH}\text{-}CO\text{-}CH_3$

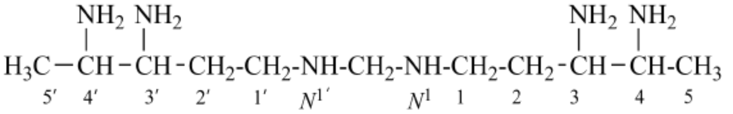
N',N'''-methylenediacetohydrazide (PIN)

P-15.3.2.2.2 In multiplicative nomenclature, a superscript arabic numeral indicating the locant of the parent structure at which the characteristic group is attached, and an appropriate number of primes, for example, N^1, $N^{2'}$, $N^{4''}$, etc., is used to distinguish among the nitrogen atoms of identical structural units containing two or more characteristic groups with one or more nitrogen atoms.

Examples:



N^1,$N^{1'}$-methylenedi(benzene-1,4-diamine) (PIN)



$H_3C-\underset{4'}{\overset{NH_2}{CH}}-\underset{3'}{\overset{NH_2}{CH}}\text{-}\underset{2'}{CH_2}\text{-}\underset{1'}{CH_2}\text{-}\underset{N^{1'}}{NH}\text{-}CH_2\text{-}\underset{N^{1}}{NH}\text{-}\underset{1}{CH_2}\text{-}\underset{2}{CH_2}\text{-}\underset{3}{\overset{NH_2}{CH}}-\underset{4}{\overset{NH_2}{CH}}\text{-}\underset{5}{CH_3}$ with H_3C numbered $5'$

N^1,$N^{1'}$-methylenedi(pentane-1,3,4-triamine) (PIN)

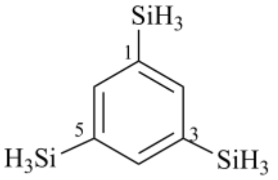
[**Note:** The attachment locant of the second of the identical parent structures is N^1; this is the locant that is primed]

For parent structures with multiple nitrogen atoms, such as di- or tricarboximidamides (P-66.4.1.4) and cyclophanamines (see P-62.2.5.3), even more complicated locant structures are required, such as primed letter locants with superscript numbers or with superscripted superscript numbers.

P-15.3.2.3 Use of multiplicative prefixes 'bis', 'tris', etc.

Identical parent structures for which the numerical prefixes 'di-', 'tri-', etc. cannot be used because of potential ambiguity (see P-16.3.6) are enclosed in parentheses or square brackets, as required, and preceded by the numerical terms 'bis-', 'tris-', etc.

Examples:



(benzene-1,3,5-triyl)tris(silane) (PIN)

(not benzene-1,3-5-triyltrisilane; trisilane is $H_3Si\text{-}SiH_2\text{-}SiH_3$)

$H_3Si\text{-}[CH_2]_{14}\text{-}O\text{-}[CH_2]_{14}\text{-}SiH_3$

[oxydi(tetradecane-14,1-diyl)]bis(silane) (PIN)

[for 'di' before 'tetradecane-14,1-diyl' see P-16.3.4 (c)]

P-15.3.2.4 Substituted identical parent structures (see P-15.3.2.1)

When identical parent structures linked by symmetrical multiplicative groups contain substituents other than a principal characteristic group, if any, on the identical parent structures, these substituent groups are cited as prefixes in one of two ways.

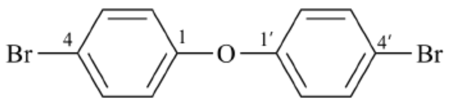
P-15.3.2.4.1 Substituent groups on the identical parent structures other than the principal characteristic group, if any, are cited as prefixes associated with the identical parent structure when they fulfill the following two conditions:

(1) the linking bonds (single or multiple) between the central substituent group of the multiplicative group and all subsequent structural units are identical; and

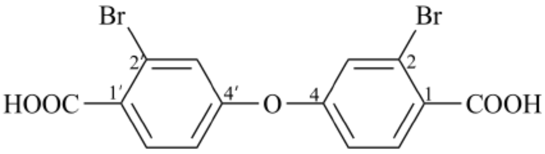
(2) the locants of all substituent groups on the identical parent structures, including suffixes, are identical.

The identical parent structures, together with their prefixes and suffixes, if any, are treated as a compound or complex group, enclosed in parentheses, square brackets, or braces according to the nesting order given in P-16.5, and designated by the appropriate numerical prefix 'bis', 'tris', 'tetrakis', etc.

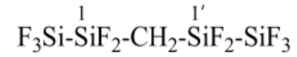
Examples:



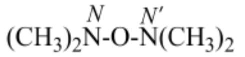
1,1′-oxybis(4-bromobenzene) (PIN)



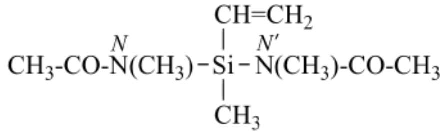
4,4′-oxybis(2-bromobenzoic acid) (PIN)


$F_3Si\text{-}\overset{1}{Si}F_2\text{-}CH_2\text{-}\overset{1'}{Si}F_2\text{-}SiF_3$

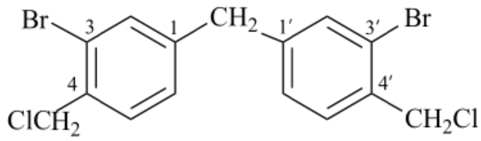
1,1′-methylenebis(pentafluorodisilane) (PIN)


$(CH_3)_2\overset{N}{N}\text{-}O\text{-}\overset{N'}{N}(CH_3)_2$

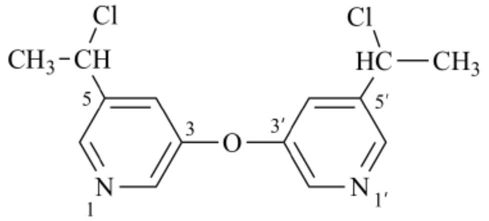
N,*N*′-oxybis(*N*-methylmethanamine) (PIN)


$CH_3\text{-}CO\text{-}\overset{N}{N}(CH_3)\text{-}\overset{CH=CH_2}{\underset{CH_3}{Si}}\text{-}\overset{N'}{N}(CH_3)\text{-}CO\text{-}CH_3$

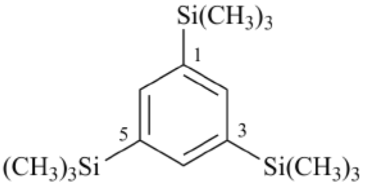
N,*N*′-[ethenyl(methyl)silanediyl]bis(*N*-methylacetamide) (PIN)



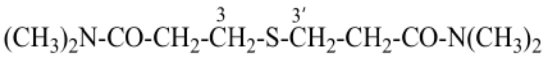
1,1′-methylenebis[3-bromo-4-(chloromethyl)benzene] (PIN)



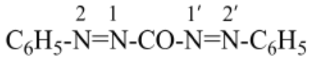
3,3′-oxybis[5-(1-chloroethyl)pyridine] (PIN)



(benzene-1,3,5-triyl)tris(trimethylsilane) (PIN)


$(CH_3)_2N\text{-}CO\text{-}CH_2\text{-}\overset{3}{C}H_2\text{-}S\text{-}\overset{3'}{C}H_2\text{-}CH_2\text{-}CO\text{-}N(CH_3)_2$

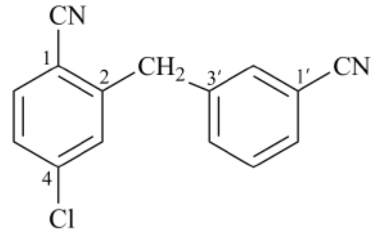
3,3′-sulfanediylbis(*N*,*N*-dimethylpropanamide) (PIN)


$C_6H_5\text{-}\overset{2}{N}=\overset{1}{N}\text{-}CO\text{-}\overset{1'}{N}=\overset{2'}{N}\text{-}C_6H_5$

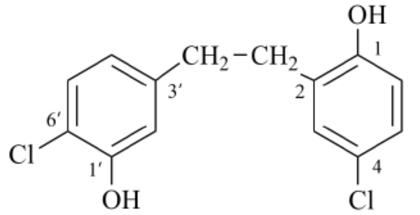
bis(phenyldiazenyl)methanone (PIN)
[not 1,1′-carbonylbis(2-phenyldiazene)]

P-15.3.2.4.2 When conditions (1) and (2) as defined in P-15.3.2.4.1, above, are not met, the substituent groups other than those identified by suffixes, if present, are cited as prefixes at the front of the name of the assembly. These prefixes are assigned the lowest locants available after priority has been given to the principal characteristic groups and the linking multiplicative substituent groups. Such names are not acceptable as preferred IUPAC names but may be used in general nomenclature; in these cases preferred IUPAC names are generated by substitutive nomenclature principles (see P-51.3.3).

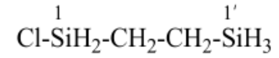
Examples:



4-chloro-2,3′-methylenedibenzonitrile (multiplicative name; numbering shown)
4-chloro-2-[(3-cyanophenyl)methyl]benzonitrile (PIN)
[not 3-[(5-chloro-2-cyanophenyl)methyl]benzonitrile;
the PIN has the greater number of substituents; see P-45.2.1)

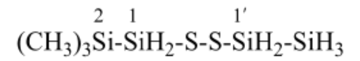


4,6′-dichloro-2,3′-(ethane-1,2-diyl)diphenol (multiplicative name; numbering shown)
4-chloro-2-[2-(4-chloro-3-hydroxyphenyl)ethyl]phenol (PIN)
[not 2-chloro-5-[2-(5-chloro-2-hydroxyphenyl)ethyl]phenol;
the locant set for the substituents in the PIN, ‘2,4’, is lower than ‘2,5’; see P-14.4 (f), P-45.2.2]



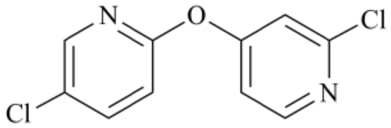
$$\overset{1}{\text{Cl-SiH}_2}\text{-CH}_2\text{-CH}_2\text{-}\overset{1'}{\text{SiH}_3}$$

1-chloro-1,1′-(ethane-1,2-diyl)bis(silane) (multiplicative name; numbering shown)
chloro(2-silylethyl)silane (PIN)
[not [2-(chlorosilyl)ethyl]silane;
the parent silane of the PIN has more substituents; see P-45.2.1]



$$(\text{CH}_3)_3\overset{2}{\text{Si}}\text{-}\overset{1}{\text{SiH}_2}\text{-S-S-}\overset{1'}{\text{SiH}_2}\text{-SiH}_3$$

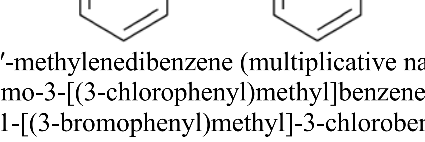
2,2,2-trimethyl-1,1′-(disulfanediyl)bis(disilane) (multiplicative name; numbering shown)
2-(disilanyldisulfanyl)-1,1,1-trimethyldisilane (PIN)
[not [2-(2,2,2-trimethyldisilan-1-yl)disulfanyl]disilane;
the parent disilane in the PIN has more substituents; see P-45.2.1)]
[not 6,6-dimethyl-3,4-dithia-1,2,5,6-tetrasilaheptane;
four heterounits are required for a skeletal replacement name (see P-51.4)]



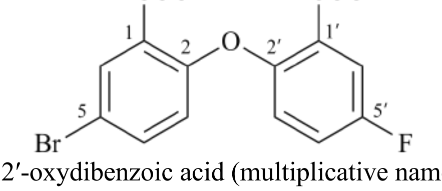
2′,5-dichloro-2,4′-oxydipyridine (multiplicative name; numbering shown)
2-chloro-4-[(5-chloropyridin-2-yl)oxy]pyridine (PIN)
[not 5-chloro-2-[(2-chloropyridin-4-yl)oxy]pyridine;
the locant set for the substituents ‘2,4’ in the PIN is lower than ‘2,5’; see P-45.2.2]

P-15.3.2.4.3 When a choice is possible, unprimed locants are assigned to the identical parent structure having the substituent cited first in alphanumerical order.

Examples:



3-bromo-3′-chloro-1,1′-methylenedibenzene (multiplicative name; numbering shown)
1-bromo-3-[(3-chlorophenyl)methyl]benzene (PIN)
[not 1-[(3-bromophenyl)methyl]-3-chlorobenzene;
‘bromochloro’ is preferred alphanumerically to ‘bromophenyl’; see P-45.5]



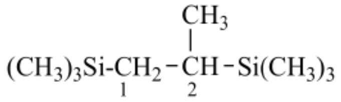
5-bromo-5′-fluoro-2,2′-oxydibenzoic acid (multiplicative name; numbering shown)

2-(4-bromo-2-carboxyphenoxy)-5-fluorobenzoic acid (PIN)
[not 5-bromo-2-(2-carboxy-4-fluorophenoxy)benzoic acid;
‘2,5’ is preferred to ‘5,2’; see P-45.2.3]

P-15.3.3 Identical units linked by unsymmetrical multiplicative groups

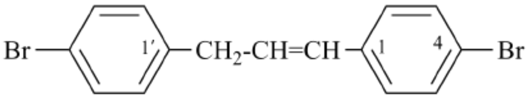
P-15.3.3.1 Unsymmetrical central multiplicative substituent groups are allowed if they are formed from a multivalent substituent group to which subsequent groups are attached by identical bonds (single or multiple). There is no limit to the number of individual groups in the full central substituent used as a multiplier.

Examples:



$$(CH_3)_3Si\text{-}\underset{1}{CH_2}-\underset{2}{\overset{\overset{\displaystyle CH_3}{|}}{CH}}-Si(CH_3)_3$$

(propane-1,2-diyl)bis(trimethylsilane) (PIN)
trimethyl[1-(trimethylsilyl)propan-2-yl]silane

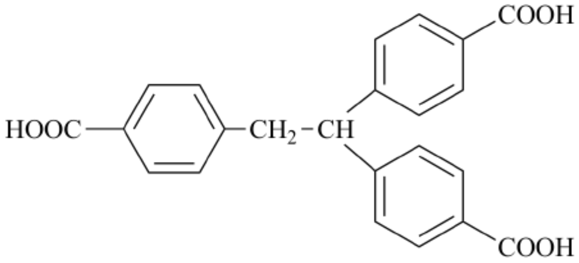


1,1′-(prop-1-ene-1,3-diyl)bis(4-bromobenzene) (PIN)
1-bromo-4-[3-(4-bromophenyl)prop-1-en-1-yl]benzene
[not 1-bromo-4-[3-(4-bromophenyl)prop-2-en-1-yl]benzene;
the correct substitutive name has lower locants in the parent substituent group]

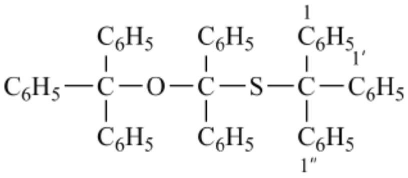
P-15.3.3.2 Choice between multiplicative names

P-15.3.3.2.1 A preferred name multiplies the most identical parent structures.

Examples:



4,4′,4″-(ethane-1,1,2-triyl)tribenzoic acid (PIN)
4,4′-[2-(4-carboxyphenyl)ethane-1,1-diyl]dibenzoic acid
(the preferred IUPAC name multiplies more identical parent structures. ‘3’ vs. ‘2’)



$$\begin{array}{ccccccccc} & & C_6H_5 & & & C_6H_5 & & & \overset{1}{C_6H_5}{}_{1'} \\ & & | & & & | & & & | \\ C_6H_5 & - & C & -O- & & C & -S- & & C-C_6H_5 \\ & & | & & & | & & & | \\ & & C_6H_5 & & & C_6H_5 & & & \underset{1''}{C_6H_5} \end{array}$$

1,1′,1″-({[diphenyl(triphenylmethoxy)methyl]sulfanyl}methanetriyl)tribenzene (PIN)
[not 1,1′-{(triphenylmethoxy)[(triphenylmethyl)sulfanyl]methylene}dibenzene;
not 1,1′,1″-({diphenyl[(triphenylmethyl)sulfanyl]methoxy}methanetriyl)tribenzene;
the preferred IUPAC name is lower alphanumerically; ‘diphenyltriphenylmethoxy’ is lower than ‘diphenyltriphenylmethyl’]

P-15.3.3.2.2 Seniority order of classes (see P-41) is used when a choice has to be made between a parent structure and a component of a multiplicative group.

Example:

$$C_6H_5\text{-}\overset{2}{N}=\overset{1}{N}\text{-CO-}\overset{1'}{N}=N\text{-}C_6H_5$$

bis(phenyldiazenyl)methanone (PIN)
[not 1,1′-carbonylbis(2-phenyldiazene);

not 1,1′-[carbonylbis(diazenediyl)]dibenzene;
ketone is senior to ‘diazene’ which is senior to the carbocycle ‘benzene’, see P-41]

P-15.3.4 Limitations of multiplicative nomenclature

Multiplicative nomenclature is not used in the following circumstances. When multiplicative nomenclature is not possible, substitutive nomenclature is used to generate preferred IUPAC names.

P-15.3.4.1 Disallowed multiplicative substituent groups
P-15.3.4.2 Disallowed identical units

P-15.3.4.1 Disallowed multiplicative substituent groups.

Three different types of multiplicative substituent groups are not allowed in multiplicative nomenclature.

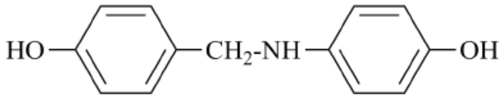
P-15.3.4.1.1 Unsymmetrical substituent groups consisting of two or more different components:

Examples:

(1) $-CH_2\text{-}OO-$ as in $H_3Si\text{-}SiH_2\text{-}CH_2\text{-}OO\text{-}SiH_2\text{-}SiH_3$

[(disilanylmethyl)peroxy]disilane (PIN)
[not [(disilanylperoxy)methyl]disilane;
‘disilanylmethylperoxy’ precedes ‘disilanylperoxymethyl’ in alphanumerical order (see P-14.5]
[not 3,4-dioxa-1,2,6,7-tetrasilaheptane;
four hetero units are required for a skeletal replacement name (see P-51.4)]

(2) $-CH_2\text{-}NH-$ as in



4-[(4-hydroxyanilino)methyl]phenol (PIN)
[not 4-{[(4-hydroxyphenyl)methyl]amino}phenol;
‘hydroxyanilinomethyl’ precedes ‘hydroxyphenylmethylamino’ in alphanumerical order (see P-14.5)]

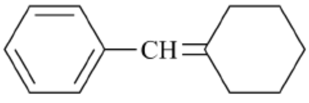
(3) $-O\text{-}CH_2\text{-}CH_2\text{-}S-$ as in $H_3Si\text{-}SiH_2\text{-}O\text{-}CH_2\text{-}CH_2\text{-}S\text{-}SiH_2\text{-}SiH_3$

3-oxa-6-thia-1,2,7,8-tetrasilaoctane (PIN)
{[2-(disilanyloxy)ethyl]sulfanyl}disilane
[not [2-(disilanylsulfanyl)ethoxy]disilane;
‘disilanyloxy’ precedes ‘disilanylsulfanyl’ in alphanumerical order; see P-14.5]

P-15.3.4.1.2 Unsymmetrical substituent groups having terminal atoms with different types of free valencies:

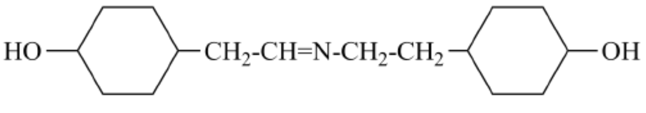
Examples:

(1) $-CH=$ as in



(cyclohexylidenemethyl)benzene (PIN)
[not (phenylmethylidene)cyclohexane; benzene is senior to cyclohexane (see P-44.4.1.1)]

(2) $-CH_2\text{-}CH=N\text{-}CH_2\text{-}CH=$ as in

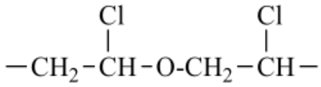


4-(2-{[2-(4-hydroxycyclohexyl)ethylidene]amino}ethylidene)cyclohexan-1-ol (PIN)
[not 4-(2-{[2-(4-hydroxycyclohexylidene)ethyl]imino}ethyl)cyclohexan-1-ol;
‘(hydroxycyclohexyl)ethylidene’ precedes ‘(hydroxycyclohexylidene)ethyl’
in alphanumerical order; see P-14.5]

P-15.3.4.1.3 Unsymmetrically substituted component units:

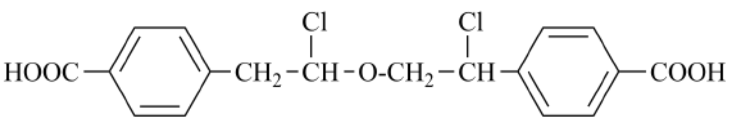
Example:

(1)



$$-CH_2-\overset{\displaystyle Cl}{\overset{|}{C}H}-O\text{-}CH_2-\overset{\displaystyle Cl}{\overset{|}{C}H}-$$

as in

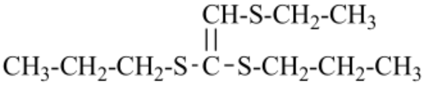


4-{2-[2-(4-carboxyphenyl)-1-chloroethoxy]-1-chloroethyl}benzoic acid (PIN)
[not 4-{2-[2-(4-carboxyphenyl)-2-chloroethoxy]-2-chloroethyl}benzoic acid;
‘1-chloroethoxy’ precedes ‘2-chloroethoxy’ in alphanumerical order; see P-45.5]

P-15.3.4.2 Disallowed identical units

Acyclic hydrocarbons, saturated or unsaturated, are not allowed as parent structures in multiplicative nomenclature [see P-15.3.1.1 (b)].

Example:



$$CH_3\text{-}CH_2\text{-}CH_2\text{-}S\text{-}\overset{\overset{\displaystyle CH\text{-}S\text{-}CH_2\text{-}CH_3}{||}}{C}\text{-}S\text{-}CH_2\text{-}CH_2\text{-}CH_3$$

1-{[2-(ethylsulfanyl)-1-(propylsulfanyl)ethen-1-yl]sulfanyl}propane (PIN; substitutive name)
(not 1,1′-{[2-(ethylsulfanyl)ethene-1,1-diyl]bis(sulfanyl)}dipropane;
alkanes are still not allowed to be identical units)

P-15.4 SKELETAL REPLACEMENT ('a') NOMENCLATURE

P-15.4.0 Introduction.

Skeletal replacement ('a') nomenclature is a subset of replacement nomenclature that also includes functional replacement nomenclature (see P-13.2). Functional replacement nomenclature is discussed in P-15.5. Just as functional replacement is considered a nomenclature, skeletal replacement is also considered a nomenclature.

In the nomenclature of organic compounds, skeletal replacement based on the replacement of carbon atoms by other atoms included in the general scope of the nomenclature of organic compounds is described under the title of skeletal replacement ('a') nomenclature, because the heteroatoms replacing carbon atoms are denoted by nondetachable prefixes ending in 'a'. Skeletal replacement ('a') nomenclature also includes replacement of boron atoms by other atoms, including carbon (see P-68.1.1.3.1), and the replacement of heteroatoms by other atoms, including carbon, to modify fundamental structures of natural products as described in P-101.4. Skeletal replacement denoted by methods other than 'a' prefixes is described for the replacement of nitrogen atoms by phosphorus and arsenic atoms in certain heterocycles (see Table 2.9) and oxygen atoms by sulfur, selenium, and tellurium atoms in other specific heterocycles (see Table 2.8).

This section deals primarily with skeletal replacement in hydrocarbon parent hydrides. Skeletal replacement ('a') nomenclature is used in two ways:

(a) to generate names for heterocyclic parent hydrides by replacing carbon atoms in corresponding cyclic hydrocarbons; and

(b) to generate simpler names for heteroacyclic structures than those formed by following the principles of substitutive nomenclature, for example, in naming polyamines, polyethers, etc., by replacing carbon atoms in corresponding acyclic hydrocarbons.

In previous recommendations, a heteroacyclic chain had to be terminated by carbon atoms (Rule R-2.2.3.1 in the 1993 Guide); but in these recommendations a heterocyclic chain now may terminate on any of the following heteroatoms: P, As, Sb, Bi, Si, Ge, Sn, Pb, B, Al, Ga, In, Tl, and C (see P-15.4.3.1).

The selection of preferred IUPAC names involving skeletal replacement ('a') nomenclature is discussed in P-51.4.

P-15.4.1 General rules

P-15.4.1.1 Nondetachable prefixes, called 'a' prefixes, are used to designate the replacing skeletal atoms with their standard bonding number. Those related to these recommendations are listed in Table 1.5.

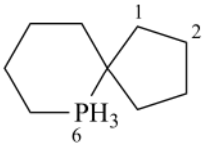
Table 1.5 Skeletal replacement ('a') prefixes

Standard Bonding Numbers	3		4		3		2		1	
	B	bora	C	carba	N	aza	O	oxa	F	fluora
	Al	alumina	Si	sila	P	phospha	S	thia	Cl	chlora
	Ga	galla	Ge	germa	As	arsa	Se	selena	Br	broma
	In	inda	Sn	stanna	Sb	stiba	Te	tellura	I	ioda
	Tl	thalla	Pb	plumba	Bi	bisma	Po	polona	At	astata

P-15.4.1.2 For naming and numbering purposes, the following decreasing order of element seniority is followed: F > Cl > Br > I >At > O > S > Se > Te > Po > N > P > As > Sb > Bi > C > Si > Ge > Sn > Pb > B > Al > Ga > In > Tl (see Appendix 1). Once a structure modified by skeletal replacement ('a') prefixes has been named and numbered, it is considered to be a new parent hydride. As locants assigned to heteroatoms are essential, all locants must be cited as defined in P-14.3.3.

P-15.4.1.3 The symbol λ^n is used to describe heteroatoms having nonstandard bonding numbers (P-14.1.3). In names, it is placed immediately after the locant (without an intervening hyphen) denoting the heteroatom.

Example:



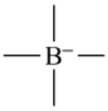
6λ^5-phosphaspiro[4.5]decane (PIN)

P-15.4.1.4 Anionic and cationic skeletal replacement ('a') prefixes used to designate anionic and cationic heteroatoms are derived from the neutral prefixes given in Table 1.5. These skeletal replacement prefixes are all preselected.

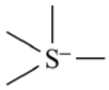
Examples:

$-P^{-}-$

phosphanida



boranuida

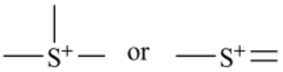


sulfanuida
λ^4-sulfanida

$-N^{+}-$

azanylia

iodonia



thionia

The selection of preferred IUPAC names involving ionic skeletal replacement ('a') prefixes is fully discussed in P-72.4 and P-73.4.

P-15.4.2 Skeletal replacement ('a') nomenclature is applied in three ways in naming heterocyclic parent hydrides.

P-15.4.2.1 Skeletal replacement ('a') nomenclature is applied simply in the generation of individual heteromonocyclic parent hydrides (see P-22.2.3), heterocyclic von Baeyer parent hydrides (see P-23.3), heterocyclic spiro parent hydrides composed of only monocyclic rings (see P-24.2.4.1), and fullerenes (see P-27.5). These heterocyclic compounds are used as identical parent structures in multiplicative nomenclature, but not as components in fusion nomenclature or ring assemblies.

P-15.4.2.2 When individual heterocycles are components of heterocyclic spiro ring systems not covered in P-15.4.2.1 above [see P-24.3.4, P-24.4.3 (in part), and P-24.5.2 (in part)], heterocyclic phane systems (see P-26.5.2), or heterocyclic ring assemblies (see P-28.4), skeletal replacement ('a') nomenclature is applied in a two-step procedure. First the structure is named as a total or partial hydrocarbon system. Then skeletal replacement ('a') prefixes are added and cited at the front of the name. Names formed by this method are used as identical parent structures in multiplicative nomenclature.

P-15.4.2.3 Heteromonocyclic mancude components named by skeletal replacement ('a') nomenclature are modified when used as component rings in fusion nomenclature [see P-25.2.2.1, P-25.2.2.4 (in part), and P-25.3.2.1.2]

P-15.4.3 Skeletal replacement ('a') nomenclature for acyclic parent hydrides

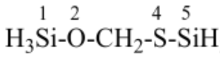
P-15.4.3.1 Skeletal replacement names are formed by placing skeletal replacement ('a') prefixes in front of the name of the unbranched parent structure in accord with their seniority order given in P-15.4.1.2. Multiplicative prefixes 'di', 'tri', 'tetra', etc, indicate a multiplicity of identical heteroatoms, and locants are used to designate their positions. The chain must be terminated by a C atom or one of the following heteroatoms: P, As, Sb, Bi, Si, Ge, Sn, Pb, B, Al, Ga, In, or Tl.

> Termination of a hetero acyclic chain by P, As, Sb, Bi, Si, Ge, Sn, Pb, B, Al, Ga, In, or Tl is a change from earlier recommendations where the chain could only be terminated by carbon atoms.

Examples:

$$\overset{1}{CH_3}\text{-}\overset{2}{O}\text{-}\overset{3}{CH_2}\text{-}\overset{4}{S}\text{-}\overset{5}{S}\text{-}\overset{6}{CH_2}\text{-}\overset{7}{CH_2}\text{-}\overset{8}{O}\text{-}\overset{9}{CH_2}\text{-}\overset{10}{CH_2}\text{-}\overset{11}{Se}\text{-}\overset{12}{CH_3}$$

2,8-dioxa-4,5-dithia-11-selenadodecane (PIN)



$$\overset{1}{\mathrm{H_3Si}}\text{-}\overset{2}{\mathrm{O}}\text{-}\mathrm{CH_2}\text{-}\overset{4}{\mathrm{S}}\text{-}\overset{5}{\mathrm{SiH_3}}$$

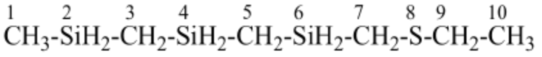
2-oxa-4-thia-1,5-disilapentane (PIN)

P-15.4.3.2 Numbering of heteroacyclic parent hydrides

P-15.4.3.2.1 Unbranched chains are numbered continuously from one end to the other so as to give a lower set of locants to heteroatoms considered together as a set without regard to kind, and then, if there is a choice, to heteroatoms cited first in the seniority order given in P-15.4.1.2.

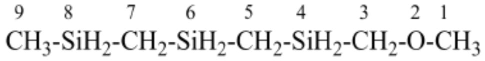
> In these recommendations, skeletal replacement ('a') nomenclature generates new acyclic parent hydrides whose numbering is fixed, as it is for rings and ring systems; this is a major modification to Rule C-0.6 (ref. 1). Then suffixes, endings, and prefixes are added in accordance with this fixed numbering.

Examples:



$$\overset{1}{\mathrm{CH_3}}\text{-}\overset{2}{\mathrm{SiH_2}}\text{-}\overset{3}{\mathrm{CH_2}}\text{-}\overset{4}{\mathrm{SiH_2}}\text{-}\overset{5}{\mathrm{CH_2}}\text{-}\overset{6}{\mathrm{SiH_2}}\text{-}\overset{7}{\mathrm{CH_2}}\text{-}\overset{8}{\mathrm{S}}\text{-}\overset{9}{\mathrm{CH_2}}\text{-}\overset{10}{\mathrm{CH_3}}$$

8-thia-2,4,6-trisiladecane (PIN)
(the locant set '2,4,6,8' is lower than '3,5,7,9'; see P-14.3.5)

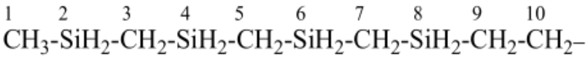


$$\overset{9}{\mathrm{CH_3}}\text{-}\overset{8}{\mathrm{SiH_2}}\text{-}\overset{7}{\mathrm{CH_2}}\text{-}\overset{6}{\mathrm{SiH_2}}\text{-}\overset{5}{\mathrm{CH_2}}\text{-}\overset{4}{\mathrm{SiH_2}}\text{-}\overset{3}{\mathrm{CH_2}}\text{-}\overset{2}{\mathrm{O}}\text{-}\overset{1}{\mathrm{CH_3}}$$

2-oxa-4,6,8-trisilanonane (PIN)
(the heteroatom locant sets, '2,4,6,8', are identical;
therefore, the low locant is given to 'O' over 'Si'; see Appendix 1)

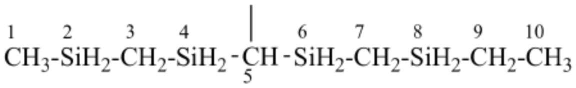
P-15.4.3.2.2 Free valences of substituent groups receive locants according to the fixed numbering of the heterochain.

Examples:



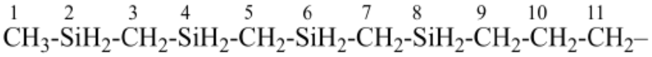
$$\overset{1}{\mathrm{CH_3}}\text{-}\overset{2}{\mathrm{SiH_2}}\text{-}\overset{3}{\mathrm{CH_2}}\text{-}\overset{4}{\mathrm{SiH_2}}\text{-}\overset{5}{\mathrm{CH_2}}\text{-}\overset{6}{\mathrm{SiH_2}}\text{-}\overset{7}{\mathrm{CH_2}}\text{-}\overset{8}{\mathrm{SiH_2}}\text{-}\overset{9}{\mathrm{CH_2}}\text{-}\overset{10}{\mathrm{CH_2}}\text{–}$$

2,4,6,8-tetrasiladecan-10-yl (preferred prefix)
[**Note** the use of 'decan-10-yl' not 'dec-10-yl'; see P-29.3.2.2]



$$\overset{1}{\mathrm{CH_3}}\text{-}\overset{2}{\mathrm{SiH_2}}\text{-}\overset{3}{\mathrm{CH_2}}\text{-}\overset{4}{\mathrm{SiH_2}}\text{-}\underset{5}{\overset{|}{\mathrm{CH}}}\text{-}\overset{6}{\mathrm{SiH_2}}\text{-}\overset{7}{\mathrm{CH_2}}\text{-}\overset{8}{\mathrm{SiH_2}}\text{-}\overset{9}{\mathrm{CH_2}}\text{-}\overset{10}{\mathrm{CH_3}}$$

2,4,6,8-tetrasiladecan-5-yl (preferred prefix)

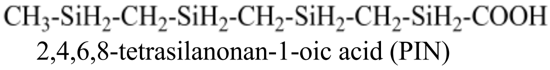


$$\overset{1}{\mathrm{CH_3}}\text{-}\overset{2}{\mathrm{SiH_2}}\text{-}\overset{3}{\mathrm{CH_2}}\text{-}\overset{4}{\mathrm{SiH_2}}\text{-}\overset{5}{\mathrm{CH_2}}\text{-}\overset{6}{\mathrm{SiH_2}}\text{-}\overset{7}{\mathrm{CH_2}}\text{-}\overset{8}{\mathrm{SiH_2}}\text{-}\overset{9}{\mathrm{CH_2}}\text{-}\overset{10}{\mathrm{CH_2}}\text{-}\overset{11}{\mathrm{CH_2}}\text{–}$$

2,4,6,8-tetrasilaundecan-11-yl (preferred prefix)

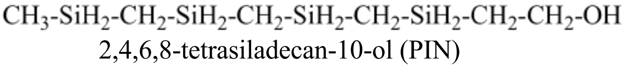
P-15.4.3.2.3 Characteristic groups cited as suffixes are given locants in accordance with the fixed numbering of the heterochain.

Examples:



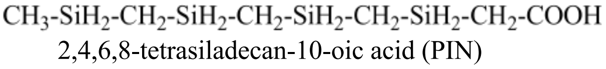
$$\overset{9}{\mathrm{CH_3}}\text{-}\overset{8}{\mathrm{SiH_2}}\text{-}\overset{7}{\mathrm{CH_2}}\text{-}\overset{6}{\mathrm{SiH_2}}\text{-}\overset{5}{\mathrm{CH_2}}\text{-}\overset{4}{\mathrm{SiH_2}}\text{-}\overset{3}{\mathrm{CH_2}}\text{-}\overset{2}{\mathrm{SiH_2}}\text{-}\overset{1}{\mathrm{C}}\mathrm{OOH}$$

2,4,6,8-tetrasilanonan-1-oic acid (PIN)
(locant 1 is not omitted, in accordance with P-15.4.3.2.1)



$$\overset{1}{\mathrm{CH_3}}\text{-}\overset{2}{\mathrm{SiH_2}}\text{-}\overset{3}{\mathrm{CH_2}}\text{-}\overset{4}{\mathrm{SiH_2}}\text{-}\overset{5}{\mathrm{CH_2}}\text{-}\overset{6}{\mathrm{SiH_2}}\text{-}\overset{7}{\mathrm{CH_2}}\text{-}\overset{8}{\mathrm{SiH_2}}\text{-}\overset{9}{\mathrm{CH_2}}\text{-}\overset{10}{\mathrm{CH_2}}\text{-OH}$$

2,4,6,8-tetrasiladecan-10-ol (PIN)



$$\overset{1}{\mathrm{CH_3}}\text{-}\overset{2}{\mathrm{SiH_2}}\text{-}\overset{3}{\mathrm{CH_2}}\text{-}\overset{4}{\mathrm{SiH_2}}\text{-}\overset{5}{\mathrm{CH_2}}\text{-}\overset{6}{\mathrm{SiH_2}}\text{-}\overset{7}{\mathrm{CH_2}}\text{-}\overset{8}{\mathrm{SiH_2}}\text{-}\overset{9}{\mathrm{CH_2}}\text{-}\overset{10}{\mathrm{C}}\mathrm{OOH}$$

2,4,6,8-tetrasiladecan-10-oic acid (PIN)

P-15.4.3.2.4 Double and triple bonds are given locants in accordance with the fixed numbering of the heterochain, and, if there is a choice, according to the general priorities for multiple bonds (see P-31.1.2.2.2).

Example:

$$\overset{1}{CH_3}\text{-}\overset{2}{SiH_2}\text{-}\overset{3}{CH_2}\text{-}\overset{4}{SiH_2}\text{-}\overset{5}{CH_2}\text{-}\overset{6}{SiH_2}\text{-}\overset{7}{CH_2}\text{-}\overset{8}{SiH_2}\text{-}\overset{9}{CH}\text{=}\overset{10}{CH_2}$$

2,4,6,8-tetrasiladec-9-ene (PIN)

P-15.4.3.2.5 Heteroatoms with nonstandard valences

(a) A nonstandard bonding number of a neutral skeletal heteroatom in a parent hydride is indicated by the symbol λ^n, where '*n*' is the bonding number following the appropriate locant (see P-14.1.3).

Example:

$$\overset{1}{CH_3}\text{-}\overset{2}{O}\text{-}\overset{3}{CH_2}\text{-}\overset{4}{CH_2}\text{-}\overset{5}{O}\text{-}\overset{6}{CH_2}\text{-}\overset{7}{CH_2}\text{-}\overset{8}{O}\text{-}\overset{9}{CH_2}\text{-}\overset{10}{CH_2}\text{-}\overset{11}{SH_2}\text{-}\overset{12}{CH_3}$$

2,5,8-trioxa-11λ^4-thiadodecane (PIN)

('O' is preferred to 'S' for low locant; see Appendix 1)

(b) When there is a choice, low locants are assigned to heteroatoms having a higher bonding number.

Example:

$$\overset{1}{CH_3}\text{-}\overset{2}{SH_2}\text{-}\overset{3}{CH_2}\text{-}\overset{4}{CH_2}\text{-}\overset{5}{S}\text{-}\overset{6}{CH_2}\text{-}\overset{7}{CH_2}\text{-}\overset{8}{S}\text{-}\overset{9}{CH_2}\text{-}\overset{10}{CH_2}\text{-}\overset{11}{S}\text{-}\overset{12}{CH_3}$$

2λ^4,5,8,11-tetrathiadodecane (PIN)

P-15.4.3.3 The use of anionic and cationic skeletal replacement ('a') prefixes is fully discussed in P-72.4 and P-73.4, respectively.

P-15.5 FUNCTIONAL REPLACEMENT NOMENCLATURE

P-15.5.1 Definition
P-15.5.2 General methodology
P-15.5.3 Scope of functional replacement nomenclature

P-15.5.1 Definition

Functional replacement nomenclature is a method by which oxygen atoms of characteristic groups and in functional parent compounds are replaced by halogen, chalcogen, and/or nitrogen atoms.

P-15.5.2 General methodology

The replacement of oxygen atoms or hydroxy groups by other atoms or groups can be described by nondetachable prefixes attached to, or infixes inserted into, names of characteristic groups, parent hydrides and functional parent compounds having retained or systematic names. A list of prefixes and infixes is given in Table 1.6. Prefixes and infixes are used for designating the replacing atom(s) –OO–, –S–, –Se–, –Te–, etc. For example, thio indicates the replacement of oxygen atoms by sulfur in the suffixes sulfonothioyl and carbothioyl and in the functional parent thioacetic acid. Similarly, peroxo or peroxy indicates the replacement of an oxygen atom by the –OO– group in the suffix peroxoic acid and in the name peroxyacetic acid. When two or more prefixes or infixes are present indicating the presence of two or more different replacement groups, they are cited in names in alphabetical order, for example, cyclohexanecarboselenothioic *S*e-acid (see P-65.1.5.1) and 3-amido-2-imidodiphosphonic chloride (see P-67.2.3).

P-15.5.3 Scope of functional replacement nomenclature

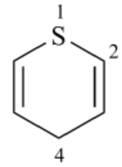
Prefixes and infixes given in Table 1.6 are used in accordance with specific rules describing replacement in:

P-15.5.3.1 Replacement in heterocyclic parent hydrides
P-15.5.3.2 Replacement in characteristic groups expressed as suffixes in substitutive nomenclature
P-15.5.3.3 Replacement in characteristic groups expressed as prefixes in substitutive nomenclature
P-15.5.3.4 Replacement in functional parent compounds

P-15.5.3.1 Replacement in heterocyclic parent hydrides

Prefixes are used to modify a limited group of parent hydrides as follows. See Table 2.2 for pyran, Table 2.3 for morpholine, Table 2.8 for chromene, isochromene and xanthene, and Table 3.1 for chromane and isochromane.

Example:



4*H*-thiopyran (PIN)
4*H*-thiine

P-15.5.3.2 Replacement in characteristic groups expressed as suffixes in substitutive nomenclature.

Replacement in suffixes is limited to –OO–, =S and –S–, =Se and –Se–, =Te and –Te–, =NH and =NNH_2 and any combination of these affixes (see Table 1.6). Suffixes including a carbon atom and those corresponding to sulfonic and sulfinic acids and their analogues are modified by infixes. Other suffixes are modified by prefixes. For examples and the order of seniority of suffixes modified by functional replacement see Tables 4.2 and 4.3 (Chapter P-4), respectively.

Table 1.6 Prefixes and infixes in functional replacement nomenclature

Prefix	Infix	Replacement atom or group	Replacing atom or group
amido	amido	–OH	$-NH_2$
azido	azido	–OH	$-N_3$
bromo	bromido	–OH	–Br
chloro	chlorido	–OH	–Cl
cyanato	cyanatido	–OH	–OCN
cyano	cyanido	–OH	–CN
dithioperoxy*	dithioperoxo*	–O–	–S-S–
fluoro	fluorido	–OH	–F
hydrazido	hydrazido	–OH	$-NH-NH_2$
hydrazono	hydrazono	=O	$=N-NH_2$
imido	imido	=O	=NH
iodo	iodido	–OH	–I
isocyanato	isocyanatido	–OH	–NCO
isocyano	isocyanido	–OH	–NC
isothiocyanato*	isothiocyanatido*	–OH	–NCS
nitrido	nitrido	=O and –OH	≡N
peroxy	peroxo	–O–	–O-O–
seleno	seleno	=O or –OH	=Se or –SeH
telluro	telluro	=O or –OH	=Te or –TeH
thio	thio	=O or –OH	=S or –SH
thiocyanato*	thiocyanatido*	–OH	–SCN
thioperoxy*	thioperoxo*	–O–	–OS– or –SO–

* Selenium and tellurium analogues are named using ‘seleno’ and ‘telluro’ in place of ‘thio’.

Examples:

–CO-OOH
carboperoxoic acid (preferred suffix)

–CO-SH
carbothioic *S*-acid (preferred suffix)

–CS-OH
carbothioic *O*-acid (preferred suffix)

–C(=NH)-OH
carboximidic acid (preferred suffix)

–SO-OOH
sulfinoperoxoic acid (preselected suffix)

$-S(=NNH_2)-OH$
sulfinohydrazonic acid (preselected suffix)

–(C)O-SH
thioic acid (preferred suffix)

–(C)S-NH_2
thioamide (preferred suffix; no contraction to thiamide)

=S
thione (preselected suffix)

–SeH
selenol (preselected suffix)

P-15.5.3.3 Replacement in characteristic groups expressed as prefixes in substitutive nomenclature

Functional replacement is used to modify prefixes containing oxygen atoms by the prefixes ‘thio’, ‘seleno’, and ‘telluro’. Prefixes are described in appropriate sections of Chapter P-6 and listed in Appendix 2.

Examples:

–C{O/S}H
thiocarboxy (preferred prefix)

=S
thioxo
sulfanylidene (preselected prefix)

P-15.5.3.4 Replacement in functional parent compounds

Functional replacement is used to modify carboxylic acids and oxoacids, by prefixes and suffixes according to specific rules given in P-15.5.3.4.1 and P-15.5.3.4.2 below. It is also used to modify two retained names expressing functional parent structures, urea and semicarbazone, as described in P-15.5.3.4.3 below. Functional replacement is not used to replace oxygen atoms in ketones, alcohols, or derivatives such as acetals and ketals, etc.; systematic names are recommended instead.

Examples:

CH_3-CS-CH_3
propane-2-thione (PIN)
(not thioacetone)

C_6H_5-SH
benzenethiol (PIN)
(not thiophenol)

P-15.5.3.4.1 In general nomenclature, retained names of monocarboxylic acids may be modified by the prefixes peroxy, thio, seleno, and telluro to indicate the replacement of an oxygen atom by the replacing atom(s) –OO–, –S– or =S, –Se– or =Se, and –Te– or =Te (see P-65.1.4.1 and P-65.1.5.2).

Examples:

CH_3-CO-SH
thioacetic *S*-acid
ethanethioic *S*-acid (PIN)

CH_3-CH_2-CS-OH
thiopropionic *O*-acid
propanethioic *O*-acid (PIN)

C_6H_5-CS-SH
dithiobenzoic acid
benzenecarbodithioic acid (PIN)

P-15.5.3.4.2 Names of mononuclear and polynuclear oxoacids are modified by prefixes and infixes listed in Table 1.6 according to the rules described in P-67.

Example:

CH_3-P(=NH)(OH)(SH)
P-methylphosphonimidothioic acid (PIN)

P-15.5.3.4.3 Retained names of acyclic polynitrogen functional parent compounds described in P-66.1.6 and P-68.3.1 are modified by prefixes ‘thio’, ‘seleno’, and ‘telluro’.

Examples:

$H_2N\text{-}CS\text{-}NH_2$
thiourea (PIN; P-66.1.6.1.3)
carbonothioic diamide

$H_2N\text{-}NH\text{-}CSe\text{-}NH_2$
selenosemicarbazide
hydrazinecarboselenoamide (PIN, see P-68.3.1.2.4)

P-15.6 CONJUNCTIVE NOMENCLATURE

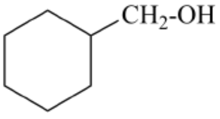
P-15.6.0 Introduction

Conjunctive nomenclature is based essentially on the conjunctive operation, by which a compound is formally constructed by subtracting the same number of hydrogen atoms from each component at each site where joined. It is traditionally reserved for naming compounds having a principal group attached to an acyclic component that is also directly attached by a carbon-carbon bond to a cyclic component. This method can be used in general nomenclature as an alternative to substitutive nomenclature, but it is not recommended for generating preferred IUPAC names (see P-51.5). The names have been modified (ref. 2) so that the placement of locants in the conjunctive names is consistent with the placement of locants in names as established in these recommendations (see P-14.3.2). Other aspects of conjunctive nomenclature used in CAS index nomenclature are discussed here briefly, including its limitations (P-15.6.2).

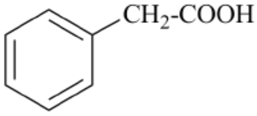
P-15.6.1 Name formation

P-15.6.1.1 Names are formed by juxtaposition of component names. The name of the cyclic component is cited first followed by the systematic or retained name of the component to which the principal characteristic group is attached.

Examples:



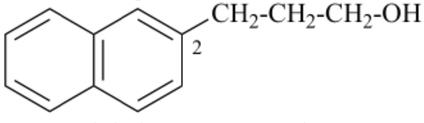
cyclohexanemethanol
cyclohexylmethanol (PIN)



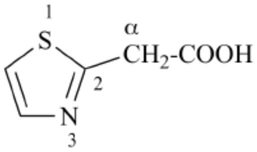
benzeneacetic acid
phenylacetic acid (PIN)

P-15.6.1.2 When necessary, the position of attachment of the side chain to the cyclic component is given by the appropriate locant placed before the name of the cyclic component, unless locants for structural features referring to the cyclic component, such as heteroatoms and indicated hydrogen, are already there; in this case the locant follows the name of the cyclic component. Since the acyclic component must terminate at the cyclic component, it is not necessary to give its locant of attachment. Carbon atoms of the side chain are indicated by Greek letters proceeding from the principal characteristic group to the cyclic component; these locants are used in the name only to locate other substituents on the side chain. The carbon atom of the characteristic group (in acids, aldehydes, nitriles, etc.) is omitted when allocating Greek letter locants.

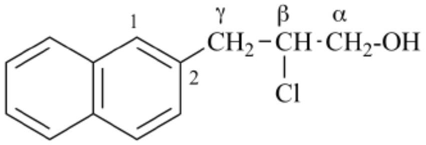
Examples:



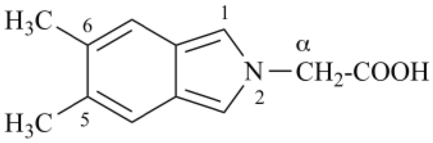
naphthalene-2-propanol
3-(naphthalen-2-yl)propan-1-ol (PIN)
3-(2-naphthyl)propan-1-ol



1,3-thiazole-2-acetic acid
(1,3-thiazol-2-yl)acetic acid (PIN)


1
γ β α
CH2-CH-CH2-OH
2
Cl

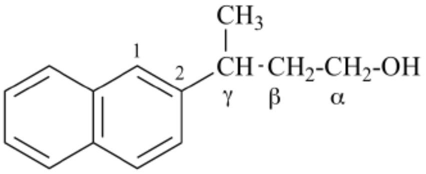
β-chloronaphthalene-2-propanol
2-chloro-3-(naphthalen-2-yl)propan-1-ol (PIN)


H3C
6
1
α
N—CH2-COOH
2
H3C
5

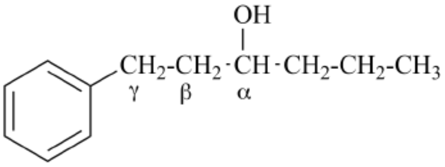
5,6-dimethyl-2*H*-isoindole-2-acetic acid
(5,6-dimethyl-2*H*-isoindol-2-yl)acetic acid (PIN)

P-15.6.1.3 For all purposes in conjunctive nomenclature the side chain is considered to extend only from the principal group to the cyclic component. Any other chain members, even those extending the side chain terminally, are named as substituents, appropriate prefixes and locants being placed before the name of the cyclic component.

Examples:


CH3
1
2
CH-CH2-CH2-OH
γ β α

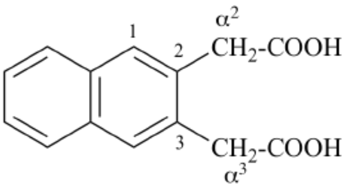
γ-methylnaphthalene-2-propanol
3-(naphthalen-2-yl)butan-1-ol (PIN)
3-(2-naphthyl)butan-1-ol


OH
CH2-CH2-CH-CH2-CH2-CH3
γ β α

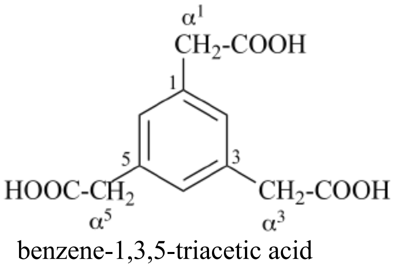
α-propylbenzenepropanol
1-phenylhexan-3-ol (PIN)

P-15.6.1.4 When a cyclic component carries at least two identical side chains, multiplicative prefixes ‘di’, ‘tri’, etc., are used to indicate their number; these prefixes are placed before the name of the side chain and superscript arabic numbers are used for all locants on the side chain instead of primes.

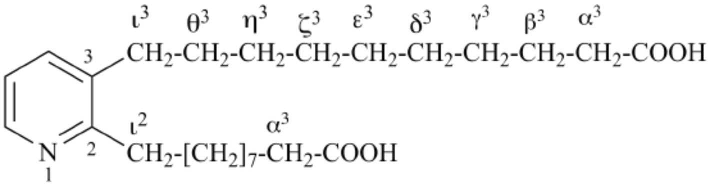
Examples:


α2
1
2
CH2-COOH
3
CH2-COOH
α3

naphthalene-2,3-diacetic acid
2,2′-(naphthalene-2,3-diyl)diacetic acid (PIN)


α1
CH2-COOH
1
5
3
HOOC-CH2
CH2-COOH
α5
α3

benzene-1,3,5-triacetic acid
2,2′,2″-(benzene-1,3,5-triyl)triacetic acid (PIN)



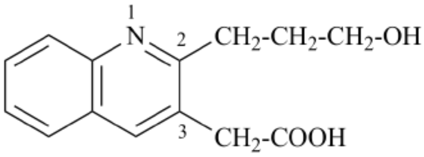
pyridine-2,3-di(decanoic acid)
10,10′-(pyridine-2,3-diyl)di(decanoic acid) (PIN)

P-15.6.1.5 When different side chains are attached to a cyclic component:

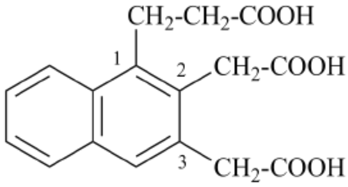
(a) the chain that contains the principal characteristic group is chosen for naming by the conjunctive method; or

(b) if there is more than one side chain containing the principal characteristic group, the conjunctive name that expresses the greater number of the principal characteristic group is chosen. When necessary, side chains are selected by applying the seniority order for selecting the principal chain (see P-44.3).

Examples:



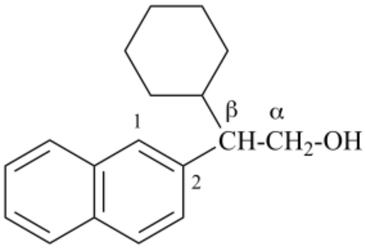
2-(3-hydroxypropyl)quinoline-3-acetic acid
[2-(3-hydroxypropyl)quinolin-3-yl]acetic acid (PIN)
(a carboxylic acid is senior to an alcohol)



1-(2-carboxyethyl)naphthalene-2,3-diacetic acid
3-[2,3-bis(carboxymethyl)naphthalen-1-yl]propanoic acid (PIN)

P-15.6.1.6 When the side chain is linked to two different cyclic components, the senior ring or ring system is selected in accord with the seniority order of rings and ring systems (see P-44.2).

Example:



β-cyclohexylnaphthalene-2-ethanol
(naphthalene is senior to cyclohexane)
2-cyclohexyl-2-(naphthalen-2-yl)ethan-1-ol (PIN)

P-15.6.2 Limitations of conjunctive nomenclature

Conjunctive nomenclature is not used when:

(a) a double bond links the acyclic component to the ring system;

(b) a double bond or a heteroatom is present in the side chain;

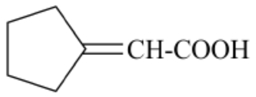
(c) two identical characteristic groups are located on the side chain provided that the condition of maximum number of principal characteristic groups is not violated;

(d) characteristic groups having higher priority for citation as principal group are directly attached to the cyclic component;

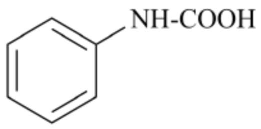
(e) two or more characteristic groups of the same kind as the principal group are located on the ring or ring system.

In the cases listed above, normal substitutive nomenclature must be used.

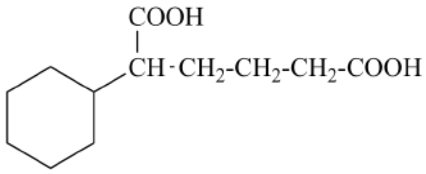
Examples:



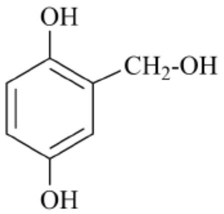
cyclopentylideneacetic acid (PIN)



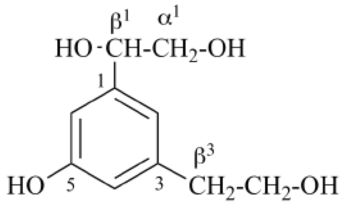
phenylcarbamic acid (PIN)



2-cyclohexylhexanedioic acid (PIN)



2-(hydroxymethyl)benzene-1,4-diol (PIN)

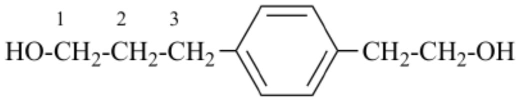


β^1,5-dihydroxybenzene-1,3-diethanol
1-[3-hydroxy-5-(2-hydroxyethyl)phenyl]ethane-1,2-diol (PIN)

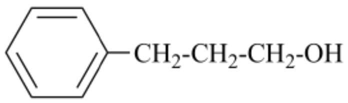
P-15.6.3 Analysis of conjunctive name construction

Note: The PIN is the substitutive name.

Example 1:



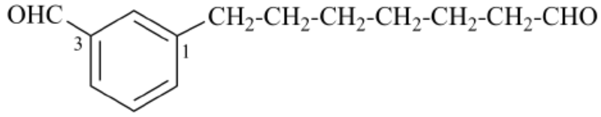
Analysis:

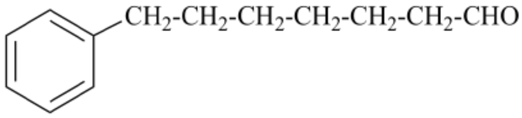
Principal group	–OH	ol
Parent:		
ring:	C_6H_6	benzene
chain:	CH_3-CH_2-CH_3	propane
Conjunctive parent including suffix:		
		benzenepropanol
Prefix:	–CH_2-CH_2-OH	
Prefix components:	–OH –CH_2-CH_3	hydroxy ethyl
Prefix name		2-hydroxyethyl

Together with other rules, this analysis leads to the conjunctive name:

4-(2-hydroxyethyl)benzenepropanol
3-[4-(2-hydroxyethyl)phenyl]propan-1-ol (PIN)

Example 2:



Principal group	–CHO	carbaldehyde or al
Parent:		
	ring	benzene
	chain	heptane
Conjunctive parent including suffix:		
		benzeneheptanal
Prefix:	–CHO	formyl

Together with other rules, this analysis leads to the conjunctive name:

3-formylbenzeneheptanal
3-(7-oxoheptyl)benzaldehyde (PIN)

P-16 NAME WRITING

P-16.0 Introduction
P-16.1 Spelling
P-16.2 Punctuation
P-16.3 Multiplicative prefixes and ‘di’, ‘tri’, etc. *vs*. ‘bis’, ‘tris, etc.
P-16.4 Other numerical terms
P-16.5 Enclosing marks
P-16.6 Italicization
P-16.7 Elision of vowels
P-16.8 Addition of vowels
P-16.9 Primes

P-16.0 INTRODUCTION

Names are written in accordance with a symbolism specific to the nomenclature of organic compounds in order to avoid ambiguity and to establish an unequivocal relationship between a name and the corresponding structure. The recommended symbolism is particularly important in the formation of IUPAC preferred names. As usual, IUPAC recognizes the needs of other languages to introduce modifications specific to a particular language, but it is hoped that, whenever possible, the following conventions will be applied to construct IUPAC names for general use as well as for IUPAC preferred names.

In the 1979 and 1993 recommendations, names were written with a capital initial letter. This practice has been abandoned in recent publications in order to ensure that names of organic compounds are not considered as proper nouns; the usual practice of capitalizing letters at the beginning of a sentence must however be respected.

P-16.1 SPELLING

The spelling of elements is that given in the IUPAC *Nomenclature of Inorganic Chemistry* (ref. 12, Table I, pp. 248-249), for example, sulfur not sulphur, aluminium not aluminum, and caesium not cesium.

P-16.2 PUNCTUATION

P-16.2.1 Commas
P-16.2.2 Full stops
P-16.2.3 Colons and semicolons
P-16.2.4 Hyphens
P-16.2.5 Spaces

P-16.2.1 Commas are used:

(a) to separate locants, numerals, or italicized letters;

Examples:

1,2-dibromoethane (PIN, P-61.3.1)
N,*N*-diethylfuran-2-carboxamide (PIN, P-66.1.1.3.1.1)

(b) to separate numbers, as well as italicized letters, in fusion descriptors when they indicate the presence of separate attached components; however, italicized letters denoting peri-fused junctions are not separated by commas.

Examples:

dibenzo[*c*,*g*]phenanthrene [PIN, P-25.3.4.2.1 (c)]
6*H*-pyrrolo[3,2,1-*de*]acridine (PIN, P-25.3.1.3)

P-16.2.2 Full stops

Full stops are used to separate numbers that denote lengths of bridges in polyalicyclic names constructed according to the von Baeyer system (see P-23.2.5.1) and of chain lengths between spiro atoms in von Baeyer spiro names (see P-24.2.1).

Examples:

bicyclo[3.2.1]octane (PIN, P-23.2.3)

6-oxaspiro[4.5]decane (PIN, P-24.2.4.1.1)

P-16.2.3 Colons and semicolons

Colons separate related sets of locants; if a higher level of separation is required, semicolons are used.

Examples:

benzo[1″,2″:3,4;4″,5″:3,4]dicyclobuta[1,2-*b*:1′,2′-*c*′]difuran (PIN, see P-25.3.7.3)
$1^1,2^1:2^2,3^1$-tercyclopropane (PIN, see P-28.3.1)

P-16.2.4 Hyphens

P-16.2.4.1 Hyphens are used in substitutive names:

(a) to separate locants from words or word fragments;

Example:

2-chloro-2-methylpropane (PIN, P-61.3.1)

(b) after parentheses, if the closing parenthesis is followed by a locant;

Examples:

1-(chloromethyl)-4-nitrobenzene (PIN, P-61.5.1)

N^1-(2-aminoethyl)-N^1,N^2,N^2-trimethylethane-1,2-diamine (PIN, P-62.2.4.1.3)

(c) to separate adjacent locants from a subsequent opening enclosing mark;

Examples:

1-(3,4-dihydroquinolin-1(2*H*)-yl)ethan-1-one (PIN, P-64.3.2)

N-acetyl-*N*-(3-chloropropanoyl)benzamide (PIN, P-66.1.2.1)

(d) to separate italic letters from Roman letters;

Examples:

di-*tert*-butyl (P-61.2.3)

as-indacene (P-25.1.1)

P-16.2.4.2 No hyphen is placed after a numerical prefix cited in front of a compound substituent enclosed by parentheses, even if that substituent begins with locants;

Example:

N,1-bis(4-chlorophenyl)methanimine (PIN, P-62.3.1.1)

P-16.2.4.3 Hyphens separate the two parts of a fusion descriptor, i.e., numbers and italicized letters.

Example:

naphtho[1,2-*a*]azulene (PIN, P-25.3.1.3)

P-16.2.4.4 Hyphens separate stereodescriptors from the rest of the name or the part of a name to which they relate.

Example:

(2*E*)-but-2-ene (PIN, P-93.4.2.1.1)

P-16.2.4.5 A long hyphen (an 'em' dash) is used to separate the names of components in adducts.

Example:

carbon monoxide—methylborane (PIN, P-13.3.5)

P-16.2.5 Spaces are a very important type of punctuation for many kinds of names in the English language. If a space is required in a name, it must be used. On the other hand, the use of spaces where they are not required, for example, in substitutive names that must be written continuously from one end to the other using hyphens to connect the different parts, may be misleading. Spaces are used in:

(a) names of acids and salts;

Examples:

acetic acid (PIN, P-65.1.1.1)

sodium 4-ethoxy-4-oxobutanoate (PIN, P-65.6.3.3.5)

(b) functional class names;

Examples:

ethyl acetate (PIN, P-65.6.3.2.1)

2-(carbonocyanidothioyl)benzoyl chloride (PIN, P-65.5.4)

butyl ethyl sulfoxide (P-63.6)
1-(ethanesulfinyl)butane (PIN)

(c) names formed using a functional modifier;

Examples:

cyclohexanone ethyl methyl ketal (P-66.6.5.1.1)
1-ethoxy-1-methoxycyclohexane (PIN)

pentan-2-one oxime (P-68.3.1.1.2)
(pentan-2-ylidene)hydroxylamine
N-hydroxypentan-2-imine (PIN)

(d) additive names;

Examples:

ethene oxide (P-63.5)
oxirane (PIN)

trimethylphosphane oxide
trimethyl-λ^5-phosphanone (PIN, P-68.3.2.3.1, P-74.2.1.4)

P-16.3 MULTIPLICATIVE PREFIXES 'DI', 'TRI', ETC. *vs.*'BIS', 'TRIS', ETC.

P-16.3.1 Multiplicative prefixes are derived from Greek and Latin number names (see P-14.2) and are the principal method for describing a multiplicity of identical features of a structure in chemical names. They are intimately interconnected with enclosing marks, particularly parentheses.

P-16.3.2 General methodology.

The general method to best determine whether 'di', 'tri', etc. or 'bis', 'tris', etc. should be used involves the following steps, not necessarily in the order given:

(a) determine whether the component to be multiplied is simple or compound. Simple components are unsubstituted parent hydrides, such as naphthalene ; unsubstituted prefixes, such as ethyl or *tert*-butyl; functionalized parent hydrides, such as benzenesulfonic acid; or retained names, such as acetic acid. All of these are multiplied by the multiplicative prefixes 'di', 'tri', etc.;

(b) determine whether these simple nomenclatural components require parentheses (see P-16.3.4) and insert them into the name;

(c) any component which is substituted automatically requires use of the multiplicative forms 'bis', 'tris', etc.;

(d) determine whether a simple nomenclature component would be ambiguous if multiplied by the multiplicative prefixes ‘di’, ‘tri’, etc., with or without the parentheses (see P-16.3.4).

P-16.3.3 The basic numerical prefixes ‘di’, ‘tri’, ‘tetra’, etc. are used to indicate a multiplicity of:

(a) functional and cumulative suffixes, basic or modified by functional replacement, with the exception of ‘thioic acid’ and ‘dithioic acid’ described in P-16.3.5 (b);

Examples:

diol (see P-63.1.2)

dicarboxylic acid (see P-65.1.1.2.1)

disulfonic acid (see P-65.3.1)

diyl (see P-71.2.3)

diide (see P-72.2.2.1)

diium (see P-73.1.1.2)

diperoxoic acid (see P-65.1.4.1)

dicarboperoxoic acid (see P-65.1 4.1)

diimidic acid (P-65.1.3.1.1)

dicarbohydrazonic acid (P-65.1.3.2.1)

disulfonoperoxoic acid (see P-65.3.1.2)

disulfinimidic acid (see P-65.3.1.4)

disulfonohydrazonimidic acid (see P-65.3.1.4)

dithioamide (see P-66.1.4.1.1)

diimidamide (see P-66.4.1.1)

dicarbohydrazonamide (P-66.4.2.1)

dicarboximidohydrazide (P-66.4.2.1)

dicarboximidamide (see P-66.4.1.1)

(b) simple substituent prefixes, including parent hydrides with ‘ene’ and ‘yne’ endings (without locants), and characteristic groups

Examples:

dicyclohexyl (see P-44.1.2)

dimethyl (see P-61.2.3)

di-*tert*-butyl (see P-61.2.3)

diethenyl (see P-61.2.3)

diimino (see P-62.3.1.2)

dibromo (see P-61.3.1)

(c) skeletal ‘a’ replacement prefixes

Examples:

trisila (see P-15.4.3.2.1)

trioxa (see P-15.4.3.2.5)

(d) multiplied components with retained names and systematic names other than those described in P-16.3.4 (c), P-16.3.4 (d) and P-16.3.4 (e).

Examples:

diphenol (see P-15.3.2.1)

diacetic acid (see P-15.3.2.1; see also P-15.6.1.4)

dipropanoic acid (see P-15.3.2.1)

(e) simple functional modifiers

Examples:

dioxime (see P-68.3.1.1.2)

dihydrazide (see P-66.3.5.2)

P-16.3.4 Parentheses (round brackets) (see P-16.6.1) are used to enclose multiplied components that are:

(a) simple substituent prefixes having locants;

Examples:

di(propan-2-yl) (preferred prefix; see P-61.2.3)

tetra(naphthalen-2-yl) (preferred prefix; see P-61.2.3)

(b) simple substituent prefixes modified by 'ene' and 'yne' endings and that have locants;

Example:

di(prop-1-en-2-yl) (preferred prefix; see P-68.2.6.1)

(c) simple substituent prefixes and functionalized parent hydrides beginning with a multiplicative prefix;

This is a change from earlier editions where 'bi' was used

Examples:

di(dodecyl) (preferred prefix; see P-68.2.6.1)

di(tridecyl) (preferred prefix, see P-52.2.8)

di(tetradecane-14,1-diyl) (multipicative preferred prefix: see P-15.3.2.1)

di(pentanal) (see P-68.2.6.2)

(d) simple substituent groups and functionalized parent hydrides beginning with 'dec' to distinguish multiplied groups from acyclic components containing 12 to 19 atoms (see P-15.1.2)

Examples:

di(decyl) (see P-57.1.1.1)

di(decanoic acid) (see P-15.3.2.1)

tri(decyl) [preferred prefix,
defines three –$C_{10}H_{21}$ groups, see P-61.2.3,
tridecyl defines the –$C_{13}H_{27}$ group, see P-57.1.1.1]

tetra(decanoic acid) (preferred suffix,
defines four decanoic acid suffixes;
tetradecanoic acid defines an acid suffix group with fourteen atoms)

(e) functionalized parent hydrides with locants;

Examples:

di(benzene-1-sulfonic acid) (see P-15.3.2.1)

di(cyclohexane-1-carboxylic acid) (see P-15.3.2.1)

(f) simple components containing brackets;

Examples:

8,8′-oxydi(spiro[4.5]decane) (PIN; see P-15.3.2.1)

di(bicyclo[3.2.1]octan-3-yl) (preferred prefix; see P-44.2.1.1)

di([4-^{2}H]benzoyl) (preferred prefix, see P-83.1.2.2)

P-16.3.5 The numerical prefixes 'bis', 'tris', 'tetrakis', etc. are used to indicate a multiplicity of:

(a) compound or complex (i.e. substituted) prefixes (see P-35.3 and P-35.4);

Examples:

bis(2-chloropropan-2-yl) (preferred prefix; see P-61.3.1)

bis(dimethylamino) (preferred prefix; see P-62.5)

ethane-1,2-diylbis(oxymethylene) (preferred prefix; see P-15.3.2.1)

bis(bromomethyl) (preferred prefix, see P-61.3.1)

(b) 'thioic acid' and 'dithioic acid' suffixes, and their Se and Te analogues, as exceptions to suffixes described in P-16.3.3 and P-16.3.4;

Examples:

bis(thioic acid) [multiple preferred suffix,
describes two –C(O/S)H suffixes, see P-65.1.5.1;
whereas dithioic acid describes a –CSSH suffix, see P-65.1.5.1]

bis(dithioic acid) (multiple preferred suffix,
describes two –CSSH suffixes, see P-65.1.5.1)
not didithoic acid

(c) before suffixes that are composed of two or more cumulative suffixes;

Examples:

bis(ylium) (multiple preferred suffix,
describes two '-ylium' suffixes, see P-73.2.2.1.2;
whereas 'diylium' could describe a cation radical suffix)

bis(nitrilium) (preferred suffix,
describes two 'nitrilium' suffixes, see P-73.1.2.1;
whereas 'dinitrilium' might be interpreted as two 'nitrile' suffixes and one 'ium' suffix)

(d) substituted functional modifiers;

Examples:

bis(phenylhydrazone) (see P-68.3.1.2.2)

pentane-2,4-dione bis(*O*-phenyloxime) (see P-68.3.1.1.2)

(e) substituted parent compounds in multiplicative nomenclature.

Examples:

bis(2-bromobenzoic acid) (see P-15.3.2.4.1)

bis[5-(1-chloroethyl)pyridine] (see P-15.3.2.4.1)

P-16.3.6 The prefixes 'bis', 'tris', 'tetrakis', etc. are also used to avoid ambiguity:

(a) before a mononuclear subset of a polynyclear acyclic structure;

Examples:

bis(sulfanyl) (preferred prefix;
defines two –SH groups, see P-63.1.5;
whereas disulfanyl defines the –SSH group; see P-63.4.2.2)

tris(sulfanyl) (preferred prefix;
defines three –SH groups (see P-63.1.5)]
whereas trisulfanyl (preferred prefix; defines the –SSSH group; see P-68.4.1)

bis(λ^4-sulfanyl) (preferred prefix;
defines two $–SH_3$ groups) (not di(λ^4-sulfanyl)

Note: And similarly for the analogous Se, Te, N, P, As, Sb, Bi, Si, Ge, Sn, Pb, B, Al, Ga, In, and Tl groups.

bis(phosphonic acid) [preselected name;
describes two phosphonic acids, see P-67.1.1.2;
diphosphonic acid describes the acid (HO)(O)PH-O-PH(O)(OH), see P-67.2.1)]

bis(hydrogen sulfate) [preselected name;
describes two (hydrogen sulfate) anions or acid esters, see P-67.1.3.2,
hydrogensulfate is an inorganic name for HSO_4^-, see ref. 12, IR 8.5]

tris(iodide) [preselected name
describes three iodide ions, see ref. 12, IR 5.4.2.3;
triiodide describes the (I_3^-) anion; see ref. 12, IR 5.4.2.3]

bis(phosphate) (preselected name)
Example: D-fructofuranose 1,6-bis(phosphate) (see P-102.5.6.1.2)]

(b) before the retained names of mononuclear divalent substituent groups, such as 'oxy', 'thio', and 'methylene' to distinguish multiplied groups from chains (see P-15.3.1.2.2.1);

Examples:

bis(oxy) [preferred prefix,
defines two –O– groups, see P-15.3.2.1;
whereas 'dioxy' would define the –OO– group, used in the past, see P-15.3.2.1)]

bis(methylene) [preferred prefix,
defines two $-CH_2-$ groups, see P-29.4.2;
whereas dimethylene might be used to define the $-CH_2$-CH_2- group
properly named as ethane-1,2-diyl (preferred prefix) or ethylene; see P-29.6.2.3]

bis(azo) defines two –N=N– groups, see P-68.3.1.3.2.3;
whereas 'diazo' is one $=N_2$ group, see P-61.4)
Example: 3,3'-[methylenebis(azo)]dipropanoic acid

bis(sulfonyl) (preferred prefix,
defines two $-SO_2-$ groups, see P-65.3.2.3;
whereas 'disulfonyl' is $-SO_2$-SO_2-)
Example: 3,3′-[oxybis(sulfonyl)]di(propan-1-ol) (PIN; see P-65.3.2.3)

bis(sulfinyl) (preferred prefix,
defines two –S(O)– groups, see P-65.3.2.3; disulfinyl is –S(O)-S(O)–)
Example: 3,3′-[azanediylbis(sulfinyl)]di(propan-1-amine) (PIN, see P-65.3.2.3)

(c) before skeletal replacement ('a') prefixes, such as 'aza', 'oxa', etc. that are used in the construction of Hantzsch-Widman names and in skeletal replacement ('a') nomenclature, to describe clearly the number of replacement atoms in a name or name component;

Examples:

benzo[1,2-*c*:3,4-*c*′]bis([1,2,5]oxadiazole) (PIN,
describes two 'oxadiazole' rings, see P-25.3.7.1;
whereas the name 'benzo[1,2-*c*:3,4-*c*′]di[1,2,5]oxadiazole' might describe
a five-membered ring with two oxygen atoms and two nitrogen atoms, see P-22.2.2.1.1)

bis(azacyclododecane) (PIN,
describes two 'azacyclododecane' rings, see P-22.2.3;
whereas the name diazacyclododecane describes
a cyclododecane ring with two nitrogen atoms, see P-22.2.3.2.2)

bis(1,2-oxazol-3-yl) [preferred prefix,
but di(isoxazol-3-yl), see P-16.3.2;
whereas di(1,2-oxazol-3-yl) might be interpreted
as a 'dioxazole' ring system, see P-22.2.2.1.1)]

(d) before attached components in fusion nomenclature to distinguish a multiplicative prefix from multiplied attached fusion components;

Examples:

bis(benzo[*a*]anthracen-1-yl) (preferred prefix,
describes two 'benzo[*a*]anthracen-1-yl prefixes; see P-61.2.4;
whereas dibenzo[*a*]anthracen-1-yl might be interpreted
as a dibenzoanthracene ring system; see P-25.3.4.2.1)

bis(cyclobuta[1,2-*c*]furan) (PIN,
describes two cyclobuta[1,2-*c*]furan ring systems, see P-25.3.7.3;

whereas dicyclobuta[1,2-*c*]furan might be interpreted
as a dicyclobutafuran ring system, see P-25.3.6.1)

(e) before names beginning with a multiplicative prefix 'di'.

Examples:

bis(diazonium) (preselected suffix, see P-73.2.2.3) (not didiazonium)

bis(diazenyl) (preselected prefix, see P-68.3.1.3.1) (not didiazenyl)

bis(disulfanyl) (preselected prefix, see P-29.3.2.2, P-63.1.5, and P-63.4.2.2) (not didisulfanyl)

tris(dihydrogen phosphate) (preselected name; see P-67.1.3.2) (not tridihydrogen phosphate)

P-16.4 OTHER NUMERICAL TERMS

P-16.4.1 The numerical prefixes 'bi', 'ter', 'quater', etc. are used mainly in naming ring assemblies (see P-28).

Examples:

1,1′-biphenyl (PIN, P-28.2.1)

$1^2,2^2{:}2^6,3^2{:}3^6,4^2$-quaterpyridine (PIN, P-28.3.1)

P-16.4.2 The prefix 'mono' is usually omitted in names of organic compounds. However, it is used to indicate that only one characteristic group of a parent structure has been modified. The ending 'kis' is never associated with 'mono'.

Examples:

monoperoxyphthalic acid (P-65.1.4.2)

2-carbonoperoxoylbenzoic acid (PIN; see P-65.1.4.2)

carbon monoxide (PIN; see P-13.3.5)

P-16.4.3 The term 'sesqui' is used to mean one and a half times as great. It is not used in IUPAC names as a numerical prefix, but may be found as a general descriptive term, for example 'sesquisiloxanes'.

P-16.5 ENCLOSING MARKS

Parentheses, ( ), (also called 'curves' or 'round brackets'), brackets, [ ], (also called 'square brackets'), and braces { }, (also called 'curly brackets') are used in chemical nomenclature to set off parts of a name dealing with specific structural features in order to convey the structure of a compound as clearly as possible. It is important to note that although they are used in the same way in names of organic and inorganic compounds, they are not used in the same way in inorganic formulas.

Enclosing marks must not be omitted from preferred IUPAC names. In general nomenclature, when there is no possible ambiguity, enclosing marks may be omitted to simplify a name.

P-16.5.1 Parentheses (also called curves or round brackets)
P-16.5.2 Brackets (also called square brackets)
P-16.5.3 Braces (also called curly brackets)
P-16.5.4 Multiple types of enclosing marks

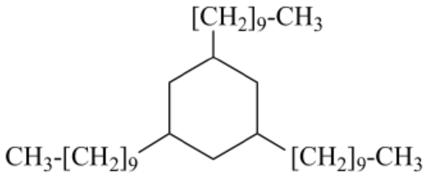
P-16.5.1 Parentheses (also called curves or round brackets)

P-16.5.1.1 Parentheses are used around compound (see P-29.1.2) and complex (see P-29.1.3) prefixes; after the multiplicative prefixes 'bis', 'tris', etc.; to enclose a multiplied parent compound consisting of a parent hydride and a substituent suffix or a multiplied substituent prefix even though preceded by a basic numerical prefix, such as 'di', 'tri', etc.

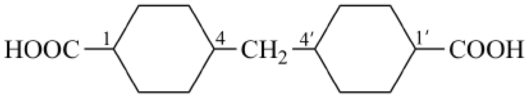
Examples:

$Cl\text{-}CH_2\text{-}SiH_3$
(chloromethyl)silane [PIN;
the name chloro(methyl)silane would describe the structure $Cl\text{-}SiH_2\text{-}CH_3$]

$(HO\text{-}CH_2\text{-}CH_2\text{-}O)_2CH\text{-}COOH$
bis(2-hydroxyethoxy)acetic acid (PIN)



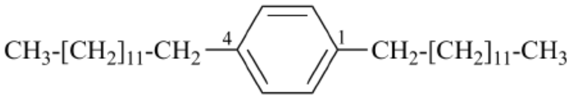
1,3,5-tri(decyl)cycohexane (PIN)
(not 1,3,5-tris(decyl)cyclohexane)



4,4′-methylenedi(cyclohexane-1-carboxylic acid) (PIN)

H{S/O}C-CH$_2$-CH$_2$-C{O/S}H
butanebis(thioic acid) (PIN)

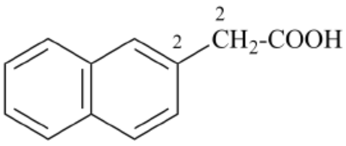
–CH-[CH$_2$]$_{12}$-CH$_2$-O-CH$_2$-[CH$_2$]$_{12}$-CH$_2$–
oxydi(tetradecane-14,1-diyl) (preferred prefix;
note the order of the substituent locants used in multiplicative nomenclature)



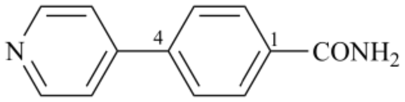
1,4-di(tridecyl)benzene (PIN)

P-16.5.1.2 Parentheses are used around simple substituent prefixes (see P-29.1) to separate locants of the same type referring to different structural elements, even though locants referring to a particular structural feature may not be explicitly cited. This is recommended for clarity since locants assigned to free valences were previously placed in front of the name, for example, 2-naphthyl.

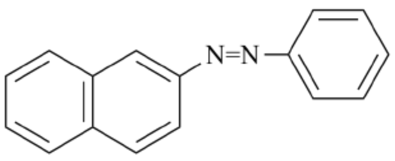
Examples:



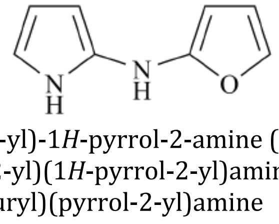
(naphthalen-2-yl)acetic acid (PIN)
(the locant ‘2’ for acetic acid is not cited, see P-14.3.4.6)
naphthalene-2-acetic acid



4-(pyridin-4-yl)benzamide (PIN)
[former name 4-(4-pyridinyl)benzamide]
4-(4-pyridyl)benzamide



(naphthalen-2-yl)(phenyl)diazene (PIN; see P-68.3.1.3.2.2)
(2-naphthyl)phenyldiazene

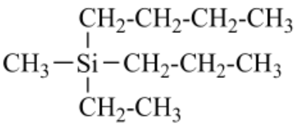


N-(furan-2-yl)-1*H*-pyrrol-2-amine (PIN)
(furan-2-yl)(1*H*-pyrrol-2-yl)amine
(2-furyl)(pyrrol-2-yl)amine

P-16.5.1.3 Parentheses for substituents of parent structures.

P-16.5.1.3.1 For mononuclear parent hydrides with two or more substituents the first cited substituent never has enclosing marks unless it a compound substituent group or includes a locant. The second and further substituents are each enclosed with parentheses even for simple substituents. When the simple substituent groups are accompanied by multiplicative prefixes such as ‘di’ and ‘tri’, the multiplicative prefixes are not included in the parentheses

Examples:

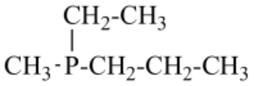


$$\begin{array}{l} \qquad\;\;\mathrm{CH_2\text{-}CH_2\text{-}CH_2\text{-}CH_3} \\ \qquad\;\;| \\ \mathrm{CH_3-Si-CH_2\text{-}CH_2\text{-}CH_3} \\ \qquad\;\;| \\ \qquad\;\;\mathrm{CH_2\text{-}CH_3} \end{array}$$

butyl(ethyl)(methyl)(propyl)silane (PIN)

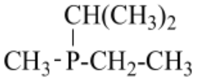
$\mathrm{CH_3\text{-}SiH_2Cl}$

chloro(methyl)silane (PIN)



$$\begin{array}{l} \qquad\;\;\mathrm{CH_2\text{-}CH_3} \\ \qquad\;\;| \\ \mathrm{CH_3\text{-}P\text{-}CH_2\text{-}CH_2\text{-}CH_3} \end{array}$$

ethyl(methyl)(propyl)phosphane (PIN)



$$\begin{array}{l} \qquad\;\;\mathrm{CH(CH_3)_2} \\ \qquad\;\;| \\ \mathrm{CH_3\text{-}P\text{-}CH_2\text{-}CH_3} \end{array}$$

ethyl(methyl)(propan-2-yl)phosphane (PIN)

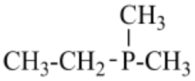
ethyl(isopropyl)(methyl)phosphane

$\mathrm{ClCH_2\text{-}SiH_2\text{-}CH_3}$

(chloromethyl)(methyl)silane (PIN; P-68.2.6.1)

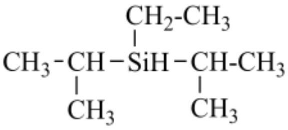
$\mathrm{BrCH_2\text{-}SiH_2\text{-}CH_2Cl}$

(bromomethyl)(chloromethyl)silane (PIN; P-68.2.6.1)



$$\begin{array}{l} \qquad\qquad\quad\mathrm{CH_3} \\ \qquad\qquad\quad| \\ \mathrm{CH_3\text{-}CH_2\text{-}P\text{-}CH_3} \end{array}$$

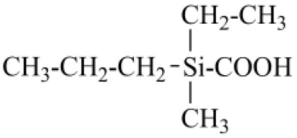
ethyldi(methyl)phosphane (PIN)



$$\begin{array}{l} \qquad\qquad\quad\mathrm{CH_2\text{-}CH_3} \\ \qquad\qquad\quad| \\ \mathrm{CH_3\text{-}CH-SiH-CH\text{-}CH_3} \\ \qquad\;\;|\qquad\qquad\;\;| \\ \qquad\mathrm{CH_3}\qquad\quad\mathrm{CH_3} \end{array}$$

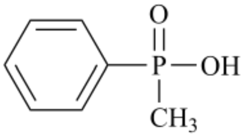
ethyldi(propan-2-yl)silane (PIN)

ethyldi(isopropyl)silane

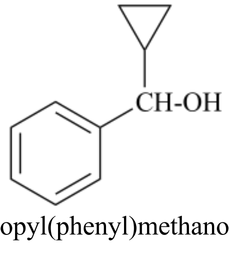


$$\begin{array}{l} \qquad\qquad\qquad\mathrm{CH_2\text{-}CH_3} \\ \qquad\qquad\qquad| \\ \mathrm{CH_3\text{-}CH_2\text{-}CH_2\text{-}Si\text{-}COOH} \\ \qquad\qquad\qquad| \\ \qquad\qquad\qquad\mathrm{CH_3} \end{array}$$

ethyl(methyl)(propyl)silanecarboxylic acid (PIN)



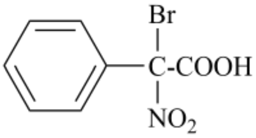
methyl(phenyl)phosphinic acid (PIN)



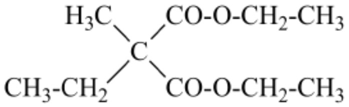
cyclopropyl(phenyl)methanol (PIN)

P-16.5.1.3.2 Simple substituents of a parent where only one possible position can be substituted do not require locants. Enclosing marks are used with second and subsequent simple substituents (see P-16.5.1.3.1). In some cases, such as acetic acid, alkyl substituents are not allowed as the resulting compound requires a different parent structure. Locants are required for related compounds where additional substitutable positions are available, for example acetamide.

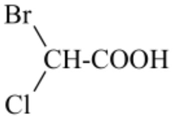
Examples:



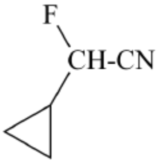
bromo(nitro)(phenyl)acetic acid (PIN)



diethyl ethyl(methyl)propanedioate (PIN)



bromo(chloro)acetic acid (PIN)

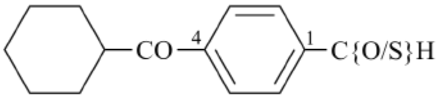


cyclopropyl(fluoro)acetonitrile (PIN)

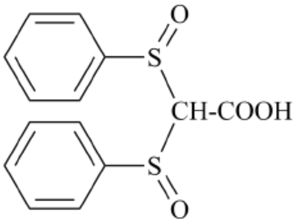
P-16.5.1.4 Parentheses are placed around substituent groups including the name of a parent hydride in order to avoid any confusion from having two parent hydrides in a substitutive name.

> This is a change from the 1993 Guide (ref. 2) to facilitate name interpretation in names as such as cyclohexanecarbonyl, in that they, even though they are simple prefixes, could give the illusion that two parent hydrides are present.

Examples:



4-(cyclohexanecarbonyl)benzene-1-carbothioic acid (PIN)



di(benzenesulfinyl)acetic acid (PIN)

P-16.5.1.5 Parentheses are placed around a prefix denoting simple hydrocarbyl substituents adjacent to the term 'amine' in naming amines using 'amine' as the parent structure, when several different substituent groups are present. This requirement is necessary to insure the specificity of this kind of amine name and to distinguish them from older names. Other enclosing marks are used as needed.

Examples:

(2-chloroethyl)(propyl)amine (P-62.2.2.1)
N-(2-chloroethyl)propan-1-amine (PIN)

butyl(ethyl)(propyl)amine (P-62.2.2.1)
N-ethyl-*N*-propylbutan-1-amine (PIN)

butyl(ethyl)(methyl)amine (P-62.2.2.1)
N-ethyl-*N*-methylbutan-1-amine (PIN)

P-16.5.1.6 Parentheses are used to isolate a second locant of a compound locant, around locants denoting ring numbering in phane nomenclature, and to enclose fullerene identifiers.

Examples:

bicyclo[8.5.1]hexadeca-1(15),10-diene (PIN, P-31.1.1.1)

1(1,3),4(1,4)-dibenzenacycloheptaphane (PIN, P-26.4.2.2)

(C_{60}-I_h)[5,6]fullerene (PIN, P-27.2.2)

P-16.5.1.7 Parentheses are used to enclose 'added indicated hydrogen' and its locant, stereodescriptors such as '*E*', '*Z*', '*R*', '*S*', etc., and descriptors for isotopically substituted compounds.

Examples:

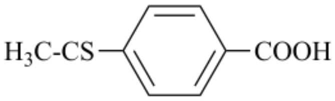
phosphinin-2(1*H*)-one (PIN, P-14.7.2)

(2*E*)-but-2-ene (PIN, P-93.4.2.1.1)

(^{13}C)methane (PIN, P-82.2.1)

P-16.5.1.8 Parentheses are used to clarify a modification made by functional replacement prefixes.

Example:



4-(thioacetyl)benzoic acid
4-(ethanethioyl)benzoic acid (PIN, P-65.1.5.1)

P-16.5.1.9 Parentheses (or other enclosing marks if parentheses are already present) are placed around a parent structure including the prefix 'di' or 'bis' before multiparent systems (P-25.3.7.1) substituted by one substituent group only cited as suffix.

Examples:

[benzo[1,2-*c*:3,4-*c*′]bis([1,2,5]oxadiazole)]-4-carboxylic acid (PIN; P-65.1.2.2.2)

(benzo[1,2:4,5]di[7]annulene)-2-carbonitrile (PIN; (P-66.5.1.1.3)

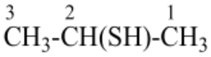
P-16.5.1.10 Parentheses are used to enclose terms modified by the numerical prefixes 'bis', 'tris', 'tetrakis', etc., discussed in P-16.3.6.

Example:

disilylmethyl (preferred prefix; see P-68.2.5)
bis(silanyl)methyl

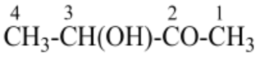
P-16.5.1.11 Parentheses are used to enclose groups attached to a chain in linear formulas.

Examples:



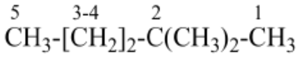
$$\overset{3}{\mathrm{C}}\mathrm{H_3}\text{-}\overset{2}{\mathrm{C}}\mathrm{H(SH)}\text{-}\overset{1}{\mathrm{C}}\mathrm{H_3}$$

propane-2-thiol (PIN)



$$\overset{4}{\mathrm{C}}\mathrm{H_3}\text{-}\overset{3}{\mathrm{C}}\mathrm{H(OH)}\text{-}\overset{2}{\mathrm{C}}\mathrm{O}\text{-}\overset{1}{\mathrm{C}}\mathrm{H_3}$$

3-hydroxybutan-2-one (PIN)



$$\overset{5}{\mathrm{C}}\mathrm{H_3}\text{-}\overset{3\text{-}4}{[\mathrm{CH_2}]_2}\text{-}\overset{2}{\mathrm{C}}\mathrm{(CH_3)_2}\text{-}\overset{1}{\mathrm{C}}\mathrm{H_3}$$

2,2-dimethylpentane (PIN)

P-16.5.1.12 Parentheses are used to enclose multiple dots and charges in radical ion structures.

Example:

$[C_6H_5\text{-}C_6H_5]^{(2\bullet)(2-)}$
[1,1′-biphenyl]dielide (PIN)
biphenyl diradical
dianion biphenyl diradical ion(2−)

P-16.5.2 Brackets (also called square brackets)

P-16.5.2.1 Brackets enclose descriptors denoting fusion sites in fused ring systems and enclose numbers denoting the length of bridges and chains connecting spiro atoms in names of polyalicyclic ring systems constructed according to von Baeyer methods. They also enclose ring assembly names when these are followed by a principal group suffix or a cumulative suffix and enclose names of components in von Baeyer spiro names.

Examples:

naphtho[2,1-*a*]azulene (PIN, P-25.3.1.3)

bicyclo[3.2.1]octane (PIN, P-23.2.2)

spiro[4.5]decane (PIN, P-24.2.1)

[2,2′-bipyridin]-5-yl (preferred prefix, P-29.3.5)

spiro[cyclohexane-1,1′-indene] (PIN, P-24.5.1)

P-16.5.2.2 Brackets enclose locants that describe structural features of components, such as double bonds in bridges and heteroatoms of component rings in names of fused ring systems.

Examples:

6,7-(epiprop[1]en[1]yl[3]ylidene)benzo[*a*]cyclohepta[*e*][8]annulene (PIN, P-25.4.3.4.2)

5*H*-pyrido[2,3-*d*][1,2]oxazine [PIN, P-25.3.2.4 (d)]

P-16.5.2.3 Brackets enclose the numerals that describe ring size in annulenes and fullerenes.

Examples:

[10]annulene (P-22.1.2)
cyclodeca-1,3,5,7,9-pentaene (PIN)

(C_{60}-I_h)[5,6]fullerene (PIN, P-27.2.2)

P-16.5.2.4 Brackets enclose substituent prefixes in which parentheses have already been used.

Example:

4-[(hydroxyselanyl)methyl]benzoic acid (PIN, P-63.4.2.2)

P-16.5.2.5 Brackets are used to enclose descriptors for isotopically labeled compounds.

Example:

[^{13}C]methane (PIN, P-83.1.2.1)

P-16.5.2.6 Brackets are employed in formulae to indicate repetition of a group in a chain.

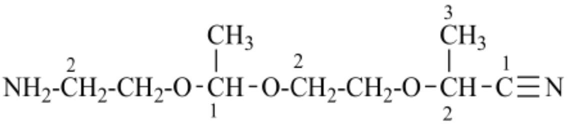
Example:

CH_3-$[CH_2]_{68}$-CH_3
heptacontane (PIN, P-21.2.1)

P-16.5.3 Braces (also called curly brackets)

P-16.5.3.1 Braces are used to enclose substituent prefixes in which brackets and parentheses have already been used.

Example:

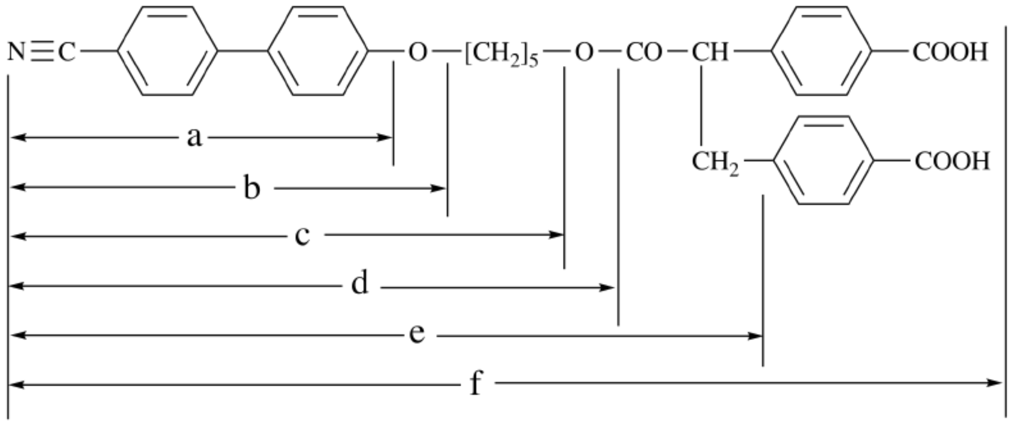


$$\mathrm{NH_2\text{-}\overset{2}{C}H_2\text{-}CH_2\text{-}O\text{-}\underset{1}{\overset{\overset{CH_3}{|}}{C}}H\text{-}O\text{-}\overset{2}{C}H_2\text{-}CH_2\text{-}O\text{-}\underset{2}{\overset{\overset{\overset{3}{CH_3}}{|}}{C}}H\text{-}\overset{1}{C}{\equiv}N}$$

2-{2-[1-(2-aminoethoxy)ethoxy]ethoxy}propanenitrile (PIN)

P-16.5.4 Multiple types of enclosing marks

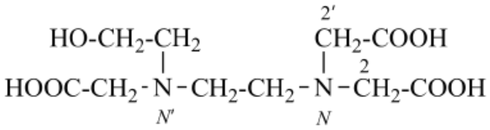
When multiple types of enclosing marks are required, the nesting order is as follows: {[({[( )]})]}, etc. as illustrated in Fig.1.3. It must be noted, however, that the presence of square brackets and/or parentheses that are an integral part of the name of a parent structure does not affect the nesting order given here.



(a) = 4′-cyano[1,1′-biphenyl]-4-yl
(b) = (4′-cyano[1,1′-biphenyl]-4-yl)oxy
(c) = 5-[(4′-cyano[1,1′-biphenyl]-4-yl)oxy]pentyl
(d) = {5-[(4′-cyano[1,1′-biphenyl]-4-yl)oxy]pentyl}oxy
(e) = 3-({5-[(4′-cyano[1,1′-biphenyl]-4-yl)oxy]pentyl}oxy)-3-oxopropane-1,2-diyl
(f) = 4,4′-[3-({5-[(4′-cyano[1,1′-biphenyl]-4-yl)oxy]pentyl}oxy)-3-oxopropane-1,2-diyl]dibenzoic acid (PIN)

Fig. 1.3 Nesting order of enclosing marks

Example:



$$\begin{matrix} & \text{HO-CH}_2\text{-CH}_2 & & \overset{2'}{\text{CH}_2}\text{-COOH} \\ & | & & |\;\;\;2 \\ \text{HOOC-CH}_2\text{-} & \underset{N'}{\text{N}} & \text{-CH}_2\text{-CH}_2\text{-} & \underset{N}{\text{N}}\text{-CH}_2\text{-COOH} \end{matrix}$$

2,2′-({2-[(carboxymethyl)(2-hydroxyethyl)amino]ethyl}azanediyl)diacetic acid
N-(carboxymethyl)-*N*′-(2-hydroxyethyl)-*N*,*N*′-(ethane-1,2-diyl)diglycine

P-16.5.4.1 The presence of square brackets and/or parentheses that are an integral part of the name of a parent structure may affect the nesting order as described below.

P-16.5.4.1.1 In determining the nesting order in a name the parentheses of added indicated hydrogen atoms are ignored.
Example:

1-(3,4-dihydroquinolin-1(2*H*)-yl)ethan-1-one (PIN, P-64.3.2)

P-16.5.4.1.2 In determining the nesting order in a name the square brackets of ring fusion, spiro fusion, ring assembly, or the extended von Baeyer names are ignored.
Examples:

(7,7-dimethyl-2-oxobicyclo[2.2.1]heptan-1-yl)methanesufonic acid (PIN, P-14.8.1)
10,10′-[[1,1′-biphenyl]-4,4′-diylbis(oxy)]di(decanoic acid) (PIN, P-15.3.2.1)
trispiro{1-oxaspiro[2.3]hexane-2,3′:4,3″:5,3‴-tri(tetracyclo[3.2.0.0^{2,7}.0^{4,6}]heptane)]}(PIN, P-24.7.4.1)
N-(dibenzo[*b*,*d*]furan-1-yl)acetamide (PIN, P-66.1.1.4.3)

P-16.5.4.1.3 In determining the nesting order in a name the parentheses used to indicate compound locants, phane amplification locants, stereochemistry, specific isotopic substitution, or coordination with multicenter bonding are taken into consideration.
Examples:

2-[bicyclo[6.6.1]pentadeca-8(15)-en-1-yl]ethan-1-ol (PIN)
trimethyl[1^2*H*-1(6)-pyrana-3,5(1,4),7(1)-tribenzenaheptaphan-7^4-yl]silane (PIN) (P-44.1.2.1)
[1(1′)*E*,3*E*,3′*E*]-3,3′-diethylidene-1,1′-bi(cyclobutylidene) (PIN, P-93.5.1.4.2.1)
[1(44)*E*,2*S*,26*R*]-bicyclo[24.20.1]heptatetraconta-1(46),44,45-trien-2-ol (PIN, P-93.5.2.3)
10-{[(3*S*)-1-phosphabicyclo[2.2.2]octan-3-yl]methyl}-10*H*-phenoxazine (PIN)
(3*S*)-2-[(2*S*)-2-{[(1*S*)-1-ethoxy-1-oxo-4-phenylbutan-2-yl]amino}propanoyl]-1,2,3,4-tetrahydroisoquinoline-3-carboxylic acid (PIN)
1,2-di[(^{13}C)methyl]benzene (PIN. P-82.2.1)
3-[ethyl(2-^{34}S)trisulfanyl]propanoic acid (PIN, P-82.6.3.2)
[(2,3,5,6-η)-bicyclo[2.2.1]hepta-2,5-diene]tricarbonyliron (P-69.2.4)
{μ-[2(1-3,3a,8a-η):1(4-6-η)]azulene}-(pentacarbonyl-1κ^{3}C,2κ^{2}C)diiron(Fe—Fe) (P-69.2.5)

P-16.5.4.1.4 In determining the nesting order where square brackets are used for an isotopically labeled compound, by convention, parentheses are used.

Example:

1-(amino[^{14}C]methyl)cyclopentan-1-ol (PIN, P-83.1.2.1)

P-16.5.4.1.5 When the nesting order given in P-16.5.4 results in consecutive enclosing marks of the same level, the next level of enclosing mark is used. For example the following name formed by the application of the nesting order rules given above results in the appearance of consecutive parentheses twice.

2-{2-[(1-ethoxy-1-oxo-4-phenylbutan-2-yl)amino]propanoyl}-1,2,3,4-tetrahydroisoquinoline-3-carboxylic acid (without stereochemistry)
(3*S*)-2-[(2*S*)-2-{[(2*S*)-1-ethoxy-1-oxo-4-phenylbutan-2-yl]amino}propanoyl]-1,2,3,4-tetrahydroisoquinoline-3-carboxylic acid (with stereochemistry)

With this example the stereochemistry needs to be inserted at three positions. Insertion of the third one into the name without stereochemistry results in two opening parenthesis next to each other. Hence to clarify the brackets these need to be adjusted as shown by the second name.

Explanation: The order of insertion of stereochemistry for 2-{2-[(1-ethoxy-1-oxo-4-phenylbutan-2-yl)amino]propanoyl}-1,2,3,4-tetrahydroisoquinoline-3-carboxylic acid is as shown below.

Stage 1 insert stereochemistry at the inner most position:

2-{2-{[(2*S*)-1-ethoxy-1-oxo-4-phenylbutan-2-yl]amino}propanoyl}-1,2,3,4-tetrahydroisoquinoline-3-carboxylic acid

The substituent (2*S*)-1-ethoxy-1-oxo-4-phenylbutan-2-yl requires square brackets to surround it hence subsequent enclosing marks need to be adjusted.

Stage 2 insert stereochemistry at the next position:

2-[(2*S*)-2-{[(2*S*)-1-ethoxy-1-oxo-4-phenylbutan-2-yl]amino}propanoyl]-1,2,3,4-tetrahydroisoquinoline-3-carboxylic acid

The substituent (2*S*)-2-{[(2*S*)-1-ethoxy-1-oxo-4-phenylbutan-2-yl]amino}propanoyl has a parenthesis on the left and brace on the right so to make clear it requires square brackets around it.

Stage 3 insert stereochemistry at the third position:

(3*S*)-2-[(2*S*)-2-{[(2*S*)-1-ethoxy-1-oxo-4-phenylbutan-2-yl]amino}propanoyl]-1,2,3,4-tetrahydroisoquinoline-3-carboxylic acid

This procedure is a change to alleviate the situation that can happen when one follows precisely the nesting order given above and it is necessary to insert independent enclosing marks to accommodate other factors, such as stereodescriptors, that two or more enclosing marks of the same type might line up consecutively resulting in confusion.

P-16.6 ITALICIZATION

Italicizing marks letters that are not involved in the primary stage of alphanumerical ordering. In manuscripts, italics are conventionally indicated by underlining when an italic font is not available.

P-16.6.1 Lower case italic letters are used in descriptors for fusion sites in names of fused ring systems.

Example:

selenopheno[2,3-*b*]selenophene (PIN, P-25.3.1.3)

The letters *o*, *m*, and *p* have been used in place of *ortho*, *meta*, and *para*, respectively, to designate the 1,2-, 1,3-, and 1,4- isomers of disubstituted benzene. This usage is strongly discouraged and is not used in preferred IUPAC names.

Example:

o-xylene (P-22.1.3)
1,2-xylene (PIN)
1,2-dimethylbenzene

P-16.6.2 Italicized elements symbols, such as *O*, *N*, *As*, are locants indicating attachment of a substituent to these heteroatoms

Examples:

N,*N*-diethylethanamine (PIN, P-62.2.2.1)

O-ethyl hexaneselenoate (PIN, P-65.6.3.3.7.1)

P-16.6.3 The italic element symbol H denotes indicated or added hydrogen.

Examples:

1*H*-azepine (PIN, P-22.2.2.1.4)
quinolin-2(1*H*)-one (PIN, P-64.3.1)

P-16.6.4 Italic terms, syllables, and capital Roman letters are used in some structural descriptors and stereodescriptors, such as '*cis*', '*trans*', '*R*', '*S*', '*E*', '*Z*', '*r*', '*s*', '*c*', '*t*', and '*retro*'.

Examples:

'*tert*', but not 'iso' (P-29.6.3)

'*E*' and '*Z*' (P-93.4.2.1.1); '*cis*', and '*trans*' (P-93.4.2.1.1); '*r*', '*c*', and '*t*' (P-93.5.1.3);

'*R*' and '*S*' (P-93.1.1), '*R**' (spoken R-star), '*S**' (spoken S-star), '*r*', '*s*', (P-93.5.1.1), '*rel*' (P-93.1.2.1)

'*meso*' (P-102.5.6.5.2), '*ambo*' (P-93.1.4), '*rac*' (P-93.1.3)

'*M*' and '*P*', 'R_a' and 'S_a', 'R_p' and 'S_p' (P-93.4.2.2 and P-93.5.5.1)

'*TPY*-3', '*TS*-3', '*SS*-4', '*TBPY*', '*SPY*', and '*OC*' (P-93.3)

'*retro*', but not 'abeo', 'apo', 'cyclo', 'de', 'des', 'homo', 'nor' or 'seco' (P-101.3.1 through P-101.3.7)

P-16.7 ELISION OF VOWELS

P-16.7.1 Vowels are systematically elided as follows:

(a) the terminal letter 'e' in names of parent hydrides or endings 'ene' and 'yne' when followed by a suffix or ending beginning with 'a', 'e', 'i', 'o', 'u', or 'y';

Examples:

pentanal (PIN, P-66.6.1.1.1)

cyclopentadec-1-en-4-yne (PIN, P-31.1.3.1)

methanium (PIN, P-73.1.1.2)

butan-2-one (PIN, P-64.2.2.1)

tetramethylboranuide (PIN, P-72.3)

sulfanyl (preselected prefix, P-29.3.1)

(b) in Hantzsch-Widman names, the final letter 'a' of an 'a' prefix when followed by a vowel;

Examples:

1,3-thiazole (PIN, P-22.2.2.1.3)
(not 1,3-thiaazaole)

1,6,2-dioxazepane (PIN, P-22.2.2.1.3)
(not 1,6,2-dioxaazaepane)

(c) the terminal letter 'a' in the names of numerical multiplicative prefixes when followed by a suffix beginning with 'a' or 'o';

Examples:

[1,1′-biphenyl]-3,3′,4,4′-tetramine (PIN, P-62.2.4.1.2)
(not [1,1′-biphenyl]-3,3′,4,4′;-tetraamine)

benzenehexol (PIN, P-63.1.2)
(not benzenehexaol)

(d) the terminal letter ‘a’ of an element ‘a’ prefix in ‘a(ba)$_n$’ repeating unit names when followed by a vowel;

Examples:

disiloxane (preselected name, P-21.2.3.1)
(not disilaoxane)

tetrastannoxane (preselected name, P-21.2.3.1)
(not tetrastannaoxane)

(e) the terminal letter ‘o’ of a functional replacement infix when followed by a vowel;

Example:

N,*P*-diphenylphosphonochloridimidic acid (PIN, P-67.1.2.4.1.1)
(not *N*,*P*-diphenylphosphonochloridoimidic acid)

(f) the terminal letter ‘o’ of ‘benzo’ in names of ‘benzoheterocycles’ formed by fusion of a benzene ring to a heteromonocycle whose name begins with a vowel [an exception to P-16.7.2 (g)].

3-benzoxepine (PIN, P-25.2.2.4)

4*H*-3,1-benzoxazine (PIN, P-25.2.2.4)

P-16.7.2 There is no elision of terminal vowels in the following cases:
(a) in conjunctive names;
Example:

benzeneacetic acid (P-15.6.1.1)
[phenylacetic acid (PIN)]

(b) from replacement or numerical multiplicative prefixes in skeletal replacement (‘a’) nomenclature;

Example:

2,4,6,8-tetrasilaundecan-11-yl (preferred prefix, P-15.4.3.2.2)

(c) from multiplicative prefixes in homogeneous acyclic parent hydrides other than hydrocarbons and boron hydrides;

Example:

nonaazane (P-21.2.2)
(not nonazane)

(d) from numerical multiplicative prefixes in multiplicative parent compounds;

Example:

2,2′,2″,2‴-(ethane-1,2-diyldinitrilo)tetraacetic acid
N,*N*′-(ethane-1,2-diyl)bis[*N*-(carboxymethyl)glycine

(e) from numerical multiplicative prefixes before substituent prefix names;

Example:

5,6,7,8-tetraiodo-1,2,3,4-tetrahydroanthracene-9-carboxylic acid (PIN, see P-65.1.2.4)

(f) from component prefixes of compound (see P-29.1.2) and complex (see P-29.1.3) prefixes before following prefixes beginning with a vowel;

Examples:

chloroamino (preselected name, P-35.3.1)

aminooxy (preselected name, P-68.3.1.1.1.5)

(g) from prefixes designating attached components in fusion nomenclature; for example, the terminal letter ‘o’ of acenaphtho, benzo, perylo, phenanthro, and the terminal letter ‘a’ of anthra, cyclopropa, cyclobuta, are not elided before a vowel [see P-16.7.1(f) for an exception involving ‘benzo’].

This recommendation is in accordance with P-25.3.1.3 and Rule R-2.4.1.1 of the 1993 Guide (ref. 2) that abrogated the elision recommended by Rule A-21.4 in the 1979 edition (ref. 1).

Examples:

cyclopropa[*de*]anthracene (PIN, P-25.3.8.1)
naphtho[1,2-*a*]azulene (PIN, P-25.3.1.3)

P-16.8 ADDITION OF VOWELS

P-16.8.1 For euphonic reasons, in functional replacement nomenclature the vowel ‘o’ is inserted between consonants.

Examples:

ethanesulfonodiimidic acid (PIN, P-65.3.1.4)
(not ethanesulfondiimidic acid)

phenylphosphononitridic acid (PIN, P-67.1.2.4.1.1)
(not phenylphosphonnitridic acid)

P-16.8.2 For euphonic reasons, the letter ‘a’ is inserted between the root of the name for polyenes, polyynes, and polyenynes, and the numerical multiplicative prefix ‘di’, ‘tri’, etc., preceding the ending ‘ene’ or ‘yne’.

Examples:

buta-1,3-diene (PIN, P-31.1.1.2)
(not but-1,3-diene)

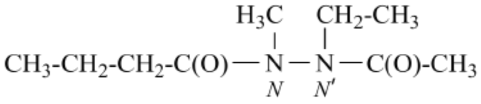
hexa-1,3-dien-5-yne (PIN, P-31.1.2.2.1)
(not hex-1,3-dien-5-yne)

P-16.9 PRIMES

In preferred IUPAC names, primes, double primes, etc., sometimes with superscripted arabic numbers that are the locants of the parent structure to which a group is attached, are added to locants and symbols without a space and are not italicized even after italic fonts. When more than three primes are required, they are cited in group of threes.

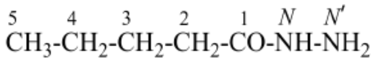
P-16.9.1 Primes (′), double primes (″), triple primes (‴), etc. are used to differentiate the nitrogen atoms of hydrazides (P-66.3), imidamides (amidines) (see P-66.4.1), hydrazonamides (amidrazones) (see P-66.4.2), and hydrazonohydrazides (hydrazidines) (see P-66.4.3).

Examples:



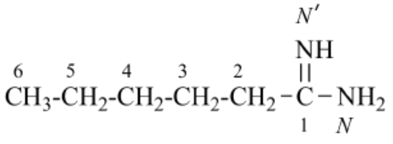
$$CH_3\text{-}CH_2\text{-}CH_2\text{-}C(O)-\underset{N}{\overset{H_3C}{N}}-\underset{N'}{\overset{CH_2\text{-}CH_3}{N}}-C(O)\text{-}CH_3$$

N′-acetyl-*N*′-ethyl-*N*-methylbutanehydrazide (PIN, P-66.3.3.2)



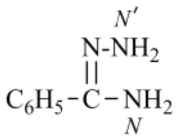
$$\overset{5}{CH_3}\text{-}\overset{4}{CH_2}\text{-}\overset{3}{CH_2}\text{-}\overset{2}{CH_2}\text{-}\overset{1}{CO}\text{-}\overset{N}{NH}\text{-}\overset{N'}{NH_2}$$

pentanehydrazide (PIN, P-66.3.1.1)



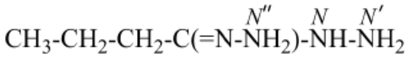
$$\overset{6}{CH_3}\text{-}\overset{5}{CH_2}\text{-}\overset{4}{CH_2}\text{-}\overset{3}{CH_2}\text{-}\overset{2}{CH_2}-\underset{1}{\overset{\overset{N'}{NH}}{\overset{||}{C}}}-\underset{N}{NH_2}$$

hexanimidamide (PIN, P-66.4.1.1)
(no longer hexanamidine)



$$C_6H_5-\overset{\overset{N'}{N\text{-}NH_2}}{\overset{||}{C}}-\underset{N}{NH_2}$$

benzenecarbohydrazonamide (PIN, P-66.4.2.1)



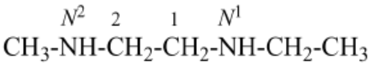
$$CH_3\text{-}CH_2\text{-}CH_2\text{-}C(=\overset{N''}{N}\text{-}NH_2)\text{-}\overset{N}{NH}\text{-}\overset{N'}{NH_2}$$

butanehydrazonohydrazide (PIN, P-66.4.3.1)

P-16.9.2 Superscript arabic numbers, which are the locants of the parent structure, are used to differentiate the nitrogen atoms of di- and polyamines, di- and polyimines, di- and polyamides, except for geminal amines, imines, and amides.

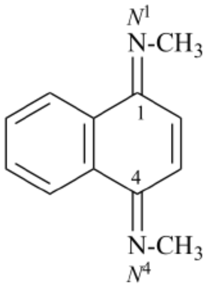
Superscript arabic numbers are now used to differentiate the nitrogen atoms of symmetrical diamines, diimines, diamides, di(imidamides), di(amidines), di(hydrazonamides), di(amidrazones), di(hydrazonohydrazides), imidohydrazides, and polyimidopolycarbonic and inorganic oxoacids, where primes (′), double primes (″), triple primes (‴), etc. were formerly used.

Examples:

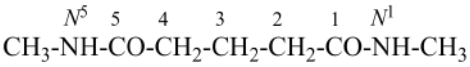


$$\overset{N^2}{CH_3}\text{-NH-}\overset{2}{CH_2}\text{-}\overset{1}{CH_2}\text{-}\overset{N^1}{NH}\text{-}CH_2\text{-}CH_3$$

*N*1-ethyl-*N*2-methylethane-1,2-diamine (PIN, P-62.2.4.1.2)
N-ethyl-*N*′-methylethane-1,2-diamine

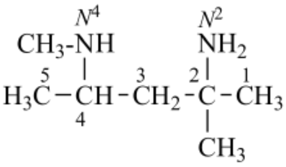


*N*1,*N*4-dimethylnaphthalene-1,4-diimine (PIN, P-62.3.1.1)
N,*N*′-dimethylnaphthalene-1,4-diimine (see also P-58.2.2.3)
N,*N*′-dimethyl-1,4-dihydronaphthalene-1,4-diimine



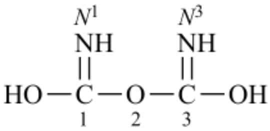
$$CH_3\text{-}\overset{N^5}{NH}\text{-}\overset{5}{CO}\text{-}\overset{4}{CH_2}\text{-}\overset{3}{CH_2}\text{-}\overset{2}{CH_2}\text{-}\overset{1}{CO}\text{-}\overset{N^1}{NH}\text{-}CH_3$$

*N*1,*N*5-dimethylpentanediamide (PIN, P-66.1.1.3.1.1)
N,*N*′-dimethylpentanediamide



$$\overset{5}{H_3C}-\underset{4}{\overset{\overset{N^4}{CH_3\text{-}NH}}{CH}}-\overset{3}{CH_2}-\underset{CH_3}{\overset{\overset{N^2}{NH_2}}{\overset{2}{C}}}-\overset{1}{CH_3}$$

*N*4,2-dimethylpentane-2,4-diamine (PIN, P-62.2.4.1.2)



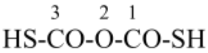
$$HO-\underset{1}{\overset{\overset{N^1}{NH}}{\overset{\|}{C}}}-\underset{2}{O}-\underset{3}{\overset{\overset{N^3}{NH}}{\overset{\|}{C}}}-OH$$

1,3-diimidodicarbonic acid (PIN, P-65.2.3.1.2.1)

Superscript arabic numbers are also used to differentiate the chalcogen atoms in polynuclear organic and inorganic oxoacids.

The use of superscripted letter locants is a change from previous practice where numerical locants were placed in front of the letter locants such as 1-*O* and 3-*O*, as described in ref. 1, Rule C-213.1.

Example:

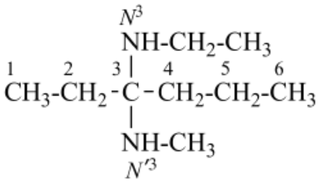


$$\overset{3}{HS}\text{-CO-}\overset{2}{O}\text{-CO-}\overset{1}{SH}$$

1,3-dithiodicarbonic *S*1,*S*3-acid
(not 1,3-dithiodicarbonic 1-*S*,3-*S*-acid)

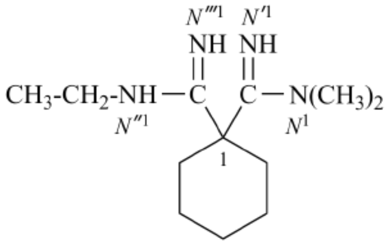
P-16.9.3 Primes (′), double primes (″), triple primes (‴), etc., with superscripted numerical locants indicating the position of the suffix on the parent structure, are used to differentiate the nitrogen atoms in cases other than those listed in P-16.9.1 and P-16.9.2, above, especially when symmetry conditions are not fulfilled.

Examples:

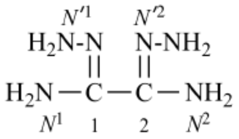


$$CH_3\text{-}CH_2\text{-}\overset{NH\text{-}CH_2\text{-}CH_3}{\underset{NH\text{-}CH_3}{C}}\text{-}CH_2\text{-}CH_2\text{-}CH_3$$

N^3-ethyl-N'^3-methylhexane-3,3-diamine (PIN, P-62.2.4.1.2)
N-ethyl-N'-methylhexane-3,3-diamine

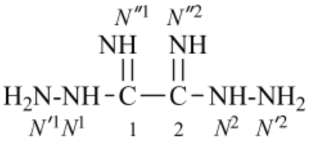


N''^1-ethyl-N^1,N^1-dimethylcyclohexane-1,1-dicarboximidamide (PIN, P-66.4.1.1 and P-66.4.1.4.2)
N''-ethyl-N,N-dimethylcyclohexane-1,1-dicarboximidamide



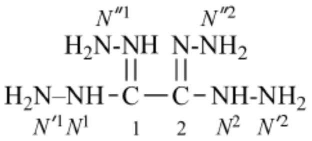
$$H_2N-\overset{H_2N\text{-}N}{\overset{\|}{C}}-\overset{N\text{-}NH_2}{\overset{\|}{C}}-NH_2$$

ethanedihydrazonamide (PIN, P-66.4.2.1)



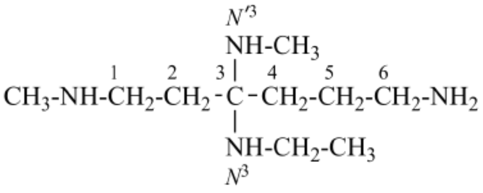
$$H_2N\text{-}NH\text{-}\overset{NH}{\overset{\|}{C}}-\overset{NH}{\overset{\|}{C}}\text{-}NH\text{-}NH_2$$

ethanediimidohydrazide (PIN, P-66.4.2.1)



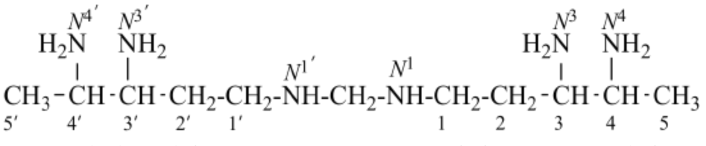
$$H_2N\text{-}NH\text{-}\overset{H_2N\text{-}NH}{\overset{\|}{C}}-\overset{N\text{-}NH_2}{\overset{\|}{C}}\text{-}NH\text{-}NH_2$$

ethanedihydrazonohydrazide (PIN, P-66.4.3.1)



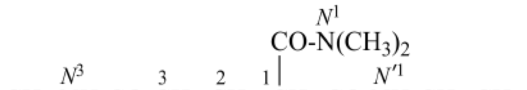
$$CH_3\text{-}NH\text{-}CH_2\text{-}CH_2\text{-}\overset{NH\text{-}CH_3}{\underset{NH\text{-}CH_2\text{-}CH_3}{C}}\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}NH_2$$

N^3-ethyl-N^1,N'^3-dimethylhexane-1,3,3,6-tetramine (PIN, P-62.2.4.1.2)
N^3-ethyl-N^1,N'^3-dimethyl(hexane-1,3,3,6-tetrayltetraamine)



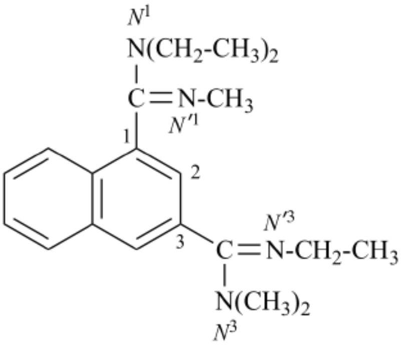
$$CH_3\text{-}\overset{H_2N}{CH}\text{-}\overset{NH_2}{CH}\text{-}CH_2\text{-}CH_2\text{-}NH\text{-}CH_2\text{-}NH\text{-}CH_2\text{-}CH_2\text{-}\overset{H_2N}{CH}\text{-}\overset{NH_2}{CH}\text{-}CH_3$$

N^1,$N^{1'}$-methylenedi(pentane-1,3,4-triamine) (PIN, P-62.2.5.2)

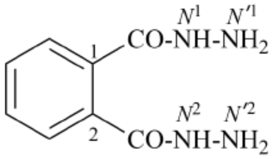


$$CH_3\text{-}NH\text{-}CO\text{-}CH_2\text{-}CH_2\text{-}\overset{CO\text{-}N(CH_3)_2}{CH}\text{-}CO\text{-}NH\text{-}CH_2\text{-}CH_3$$

N'^1-ethyl-N^1,N^1,N^3-trimethylpropane-1,1,3-tricarboxamide (PIN, P-66.1.1.3.1.2)



N^1,N^1,N'^3-triethyl-N'^1,N^3,N^3-trimethylnaphthalene-1,3-dicarboximidamide (PIN, P-66.4.1.4.1)



benzene-1,2-dicarbohydrazide (PIN, P-66.3.1.2.2)

P-16.9.4 Primes (′), double primes (″), triple primes (‴), etc., are also used to differentiate identical locants other than *N* locants, for example 1, 1′, 1″, 4′a (not 4a′; for locants of a fused ring component, primes are added after the number, not after the letter). Such usage occurs:

(a) in multiplicative nomenclature to denote multiplied units and modify locants accordingly;

Example:

2,2′,2″-nitrilotri(ethan-1-ol) (PIN, P-15.3.2.1)

(b) in spiro-fused compounds, to denote positions in polycyclic systems, identical or different;

Examples:

7,7′-spirobi[bicyclo[4.1.0]heptane] (PIN, P-24.3.1)

1*H*,1′*H*,1″*H*,3′*H*-2,2′:7′,2″-dispiroter[naphthalene] (PIN, P-24.4.1)

spiro[cyclohexane-1,1′-indene] (PIN, P-24.5.1)

(c) in ring assemblies, to number identical ring components;

Examples:

1,1′-bi(cyclopropane) (PIN, P-28.2.1)

1,1′-biphenyl (PIN, P-28.2.1)

3a,3′a-biindene (PIN, P-28.2.3)

P-16.9.5 Primes also occur:

(a) in fusion nomenclature, to identify first and higher attached components, identical attached components, and multiparent names;

Examples:

pyrido[1″,2″:1′,2′]imidazo[4′,5′:5,6]pyrazino[2,3-*b*]phenazine (PIN, P-25.3.4.1.1)

difuro[3,2-*b*:2′,3′-*e*]pyridine (PIN, P-25.3.4.1.2)

cyclopenta[1,2-*b*:5,1-*b*′]bis([1,4]oxathiine) (PIN, P-25.3.7.1)

(b) in fullerenes *ortho*-fused to organic ring or ring systems, to identify positions in the nonfullerene component;

Example:

3′*H*-cyclopropa[1,9](C_{60}-I_h)[5,6]fullerene (PIN, P-27.6.1)

(c) in natural product nomenclature, to identify positions in ring(s) fused to a fundamental parent hydride;

Example:

naphtho[2′,1′:2,3]-5α-androstane (P-101.5.1.1)

P-16.9.6 Multiple primes

Long strings of primes may be needed with ring assemblies and polyspiro compound. It is difficult to count long streams of primes. For example, how many primes appear in this string: ′′′′′′′′? It is eight. In these recommendations, to simplify the counting process, long strings of primes are broken into groups of three as: ′′′ ′′′ ′′, which has the same number of primes as the string above. This is a change from the publication on spiro compounds (ref. 8) in which multiple primes were separated by a space after every four primes.

International Union of Pure and Applied Chemistry

Division VIII Chemical Nomenclature and Structure Representation Division

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Chapter P-2 PARENT HYDRIDES

P-20 Introduction
P-21 Mononuclear and acyclic polynuclear parent hydrides
P-22 Monocyclic parent hydrides
P-23 Polyalicyclic parent hydrides (extended von Baeyer system)
P-24 Spiro ring systems
P-25 Fused and bridged fused ring systems
P-26 Phane nomenclature
P-27 Fullerenes
P-28 Ring assemblies
P-29 Prefixes denoting substituent groups derived from parent hydrides

P-20 INTRODUCTION

A parent hydride is the structure that is named before the addition of affixes denoting substituents to yield the name of a specific compound. Its name is understood to signify a definite population of hydrogen atoms attached to a skeletal structure. Acyclic parent hydrides are always saturated and unbranched, for example, pentane and trisilane. Cyclic parent hydrides are usually either fully saturated, for example, cyclopentane, cyclotrisiloxane, azepane, bicyclo[3.2.1]octane, and spiro[4.5]decane, or fully unsaturated, i.e., they contain the maximum number of noncumulative double bonds, for example benzene, pyridine, 1,3-oxazole, 1*H*-phenalene, phenanthroline, and benzo[*a*]acridine. Also, there are parent hydrides that are partially saturated, for example 1*H*-spiro[[1,3]-dioxolane-2,1′-indene], and there are combinations of cyclic and acyclic hydrides, having traditional retained names, for example toluene.

Names of parent hydrides that do not contain skeletal carbon atoms, for example trisilane, are not designated as preferred IUPAC names in these recommendations. Instead they are called preselected names, i.e., they are used to generate preferred IUPAC names for derivatives substituted by organic (carbon-containing) substituents (see P-12.2). They may, however, become IUPAC preferred names depending on decisions of a team formed to decide IUPAC preferred names for inorganic (noncarbon-containing) compounds.

Names of parent hydrides are either traditional names that are retained or systematic names formed in accordance with specific rules. Rules and names must be unambiguous and clear. In order to achieve this goal and keep rules simple and concise, the rules for selecting preferred IUPAC names and preselected names of parent hydrides and prefixes denoting substituent groups derived from parent hydrides are not provided in this Chapter. These rules are given in Chapter P-5.

P-21 MONONUCLEAR AND ACYCLIC POLYNUCLEAR PARENT HYDRIDES

P-21.1 Mononuclear parent hydrides
P-21.2 Acyclic polynuclear parent hydrides

P-21.1 MONONUCLEAR PARENT HYDRIDES

P-21.1.1 Mononuclear parent hydrides with standard bonding numbers

P-21.1.1.1 Systematic names

The names of mononuclear hydrides of the elements for use as parents in naming organic compounds by substitutive nomenclature are given in Table 2.1. Most are formed systematically by citing the ‘a’ term of the element (see Table 2.4) with elision of the terminal letter ‘a’ before the ending ‘ane’ (patterned after methane), for example borane for BH_3 and silane for SiH_4, etc. There are important exceptions: oxidane for H_2O, sulfane for H_2S, selane for H_2Se, tellane for H_2Te, polane for H_2Po, and bismuthane for BiH_3 (see Table 2.1). The systematically formed names oxane, thiane, selenane, tellurane, polonane, and bismane are Hantzsch-Widman names designating the corresponding saturated six-membered rings with a single heteroatom. The name ‘carbane’ has never been used in place of methane; it is not recommended.

Table 2.1 Systematic names of mononuclear parent hydrides of the elements in Groups 13, 14, 15, 16, and 17 with normal bonding numbers

(all systematic names, except for carbane, are preselected names; see P-12.2; for the retained name methane, see P-21.1.1.2)

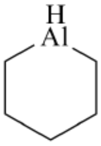
Groups	**13**	**14**	**15**	**16**	**17**
	BH_3 borane	CH_4 (carbane)*	NH_3 azane	OH_2 oxidane	FH fluorane
	AlH_3 alumane	SiH_4 silane	PH_3 phosphane	SH_2 sulfane	ClH chlorane
	GaH_3 gallane	GeH_4 germane	AsH_3 arsane	SeH_2 selane	BrH bromane
	InH_3 indigane	SnH_4 stannane	SbH_3 stibane	TeH_2 tellane	IH iodane
	TlH_3 thallane	PbH_4 plumbane	BiH_3 bismuthane	PoH_2 polane	AtH astatane

* Note that methane is the preferred IUPAC name.

See P-21.1.1.2 for common names used in the IUPAC nomenclature of organic and inorganic compounds.

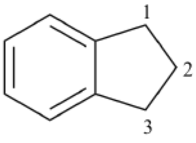
The newly recommended names gallane and thallane are formed systematically. Alumane and indigane are exceptions. The name 'aluminane' could be ambiguous as it could designate the mononuclear hydride AlH_3 and the saturated six-membered ring with one aluminium atom that has a Hantzsch-Widman name denoted by the ending '-inane'. The name 'alane' has been used, but must also be discarded because its systematically derived substituent group, $H_2Al–$, would be named 'alanyl', the well entrenched name for the acyl group derived from the amino acid alanine. The name alumane has no negative connotation. The prefix 'aluma' is recommended for forming Hantszch-Widman names, and thus the name 'aluminane' describes the saturated six-membered ring monocycle containing one aluminium atom (see P-22.2.2). The systematically formed name 'indane' cannot be used because it is already used to designate a partially saturated bicyclic fused hydrocarbon. Reich and Richter (ref. 20) called the element indium in 1863 after the indigo colored flame test, recognized as different than the color from caesium. Returning to the source indigo, 'indigane' could be an acceptable name; it is thus recommended for the hydride InH_3.

AlH_3
alumane (preselected name, see P-12.2)
(not alane)



aluminane

InH_3
indigane (preselected name, see P-12.2)



indane
2,3-dihydro-1*H*-indene (PIN)

The monohydride names listed in Table 2.1 constitute the basis of 'generalized ane nomenclature'. Substitutive nomenclature as applied to alkanes, cycloalkanes, and polycycloalkanes has been systematically extended to hydrides of elements of Groups 13, 14, 15, 16, and 17. Generalized 'ane' nomenclature is divided into 'carbane nomenclature', which covers the traditional substitutive nomenclature for carbon parent hydrides, and 'heterane nomenclature', which relates to atoms other than carbon, referred to as heteroatoms.

P-21.1.1.2 Retained names

The common name methane is retained. The common names water, ammonia, the binary names for the hydracids of Group 17, for example hydrogen chloride, and binary names for the hydrides of Group 16, for example hydrogen sulfide, are used in these recommendations but their use as preferred IUPAC names is deferred pending publication of recommendations for the selection of preferred inorganic names; thus, no PIN label will be assigned in names including them (see P-14.8). However, systematic alternatives to these common names, e.g. oxidane for water and azane for ammonia, and for the binary names of hydracids of Group 17 and the hydrides of Group 16, for example chlorane for hydrogen chloride and sulfane for hydrogen sulfide, are necessary for naming some derivatives and for generating names of radicals, ions, and polynuclear homologues.

The names ‘phosphine’ for PH_3, ‘arsine’ for AsH_3, ‘stibine’ for SbH_3, and ‘bismuthine’ for BiH_3, are retained for use in general nomenclature.

P-21.1.2 Mononuclear parent hydrides with nonstandard bonding numbers

P-21.1.2.1 Systematic and traditional names

If the bonding number of the element differs from the standard one as defined in P-14.1 and exemplified in Table 2.1, the name of the hydride is modified by affixing the symbol λ^n, where ‘*n*’ is the bonding number, to the name of the hydride (ref. 13).

The names ‘phosphorane’ for PH_5, ‘arsorane’ for AsH_5, and ‘stiborane’ for SbH_5, are retained for use in general nomenclature. However, the names ‘sulfurane’ for SH_4, ‘selenurane’ for SeH_4, ‘iodinane’ for IH_3, ‘persulfurane’ for SH_6, and ‘periodinane’ for IH_5, which have been used in recent literature, are not recommended.

Examples:

IH_3
λ^3-iodane (preselected name, see P-12.2)
(not iodinane)

SH_4
λ^4-sulfane (preselected name, see P-12.2)
(not sulfurane)

SnH_2
λ^2-stannane (preselected name, see P-12.2)

PH_5
λ^5-phosphane (preselected name, see P-12.2)
phosphorane

AsH_5
λ^5-arsane (preselected name, see P-12.2)
arsorane

SbH_5
λ^5-stibane (preselected name, see P-12.2)
stiborane

P-21.2 ACYCLIC POLYNUCLEAR PARENT HYDRIDES

P-21.2.1 Hydrocarbons
P-21.2.2 Homogeneous acyclic parent hydrides other than hydrocarbons and boron hydrides
P-21.2.3 Heterogenous acyclic parent hydrides
P-21.2.4 Acyclic parent hydrides containing heteroatoms with nonstandard bonding numbers

P-21.2.1 Hydrocarbons

The saturated unbranched acyclic hydrocarbons C_2H_6, C_3H_8, and C_4H_{10} have the retained names ethane, propane, and butane, respectively. Systematic names for the higher members of this series consist of a numerical term (see Table 1.4) followed by the ending ‘ane’ with elision of the terminal letter ‘a’ from the numerical term. The generic name for saturated acyclic hydrocarbons (branched or unbranched) is ‘alkane’. The chain is numbered from one end to the other with arabic numbers. Brackets are employed in formulas to indicate repetition of groups in chains. For unsaturated acyclic hydrocarbons see P-31.1.

Examples:

$$\overset{7}{CH_3}\text{-}\overset{6}{CH_2}\text{-}\overset{5}{CH_2}\text{-}\overset{4}{CH_2}\text{-}\overset{3}{CH_2}\text{-}\overset{2}{CH_2}\text{-}\overset{1}{CH_3}$$

heptane (PIN)

$$\overset{20}{CH_3}\text{-}[CH_2]_{18}\text{-}\overset{1}{CH_3}$$

icosane (PIN)
(the Beilstein and CAS index name is ‘eicosane’)

$$\overset{23}{C}H_3\text{-}[CH_2]_{21}\text{-}\overset{1}{C}H_3$$

tricosane (PIN)

$$\overset{70}{C}H_3\text{-}[CH_2]_{68}\text{-}\overset{1}{C}H_3$$

heptacontane (PIN)

P-21.2.2 Homogeneous acyclic parent hydrides other than hydrocarbons and boron hydrides

A compound consisting of an unbranched chain containing two or more identical heteroatoms saturated with hydrogen atoms is named by citing the appropriate multiplying prefix from Table 1.4 (with no elision of the terminal vowel of the multiplying prefix) followed by the name of the appropriate hydride according to P-21.1. These names are preselected (see P-12.2). Potential functionality of terminal groups, such as –SH or –OH, is ignored.

Examples:

$$\overset{2}{N}H_2\text{-}\overset{1}{N}H_2$$

hydrazine (retained, preselected name, see P-12.3)
diazane

$$\overset{9}{N}H_2\text{-}[NH]_7\text{-}\overset{1}{N}H_2$$

nonaazane (preselected name, see P-12.2)

$$\overset{5}{Si}H_3\text{-}\overset{4}{Si}H_2\text{-}\overset{3}{Si}H_2\text{-}\overset{2}{Si}H_2\text{-}\overset{1}{Si}H_3$$

pentasilane (preselected name, see P-12.2)

$$\overset{5}{P}H_2\text{-}\overset{4}{P}H\text{-}\overset{3}{P}H\text{-}\overset{2}{P}H\text{-}\overset{1}{P}H_2$$

pentaphosphane (preselected name, see P-12.2)

HS-S-S-SH
tetrasulfane (preselected name)
(not disulfanedithiol nor trisulfanethiol, see P-58.3.1)

P-21.2.3 Heterogeneous acyclic parent hydrides. There are two types to be considered.

P-21.2.3.1 Heterogeneous parent hydrides composed of alternating atoms
P-21.2.3.2 Heterogeneous parent hydrides formed by skeletal replacement (‘a’) nomenclature

P-21.2.3.1 Heterogeneous parent hydrides composed of alternating heteroatoms, i.e., [a(ba)$_n$ hydrides], excluding carbon atoms and the halogen atoms

Compounds containing an unbranched chain of alternating atoms terminated by two identical atoms of the element coming later in the seniority order O > S > Se > Te > N > P >As > Sb > Bi > Si > Ge > Sn > Pb > B >Al > Ga > In > Tl maybe named by citing successively a multiplying prefix denoting the number of atoms of the terminal element followed by the ‘a’ term for that element, then the ‘a’ term of the other element in the chain and the ending ‘ane’. The terminal letter ‘a’ of an ‘a’ term is elided when followed by a vowel; the terminal vowel of a numerical prefix is not elided even when the ‘a’ term begins with the same vowel. When nitrogen atoms are present, amine names (see P-62) should be used because of the higher functionality of amines. This concept does not extend to other elements. These parent hydrides are preselected parent hydrides (see P-12.2) and have priority to receive preferred IUPAC names, as long as they are used to name compounds containing carbon.

This is a change from the 1993 Guide (ref. 2) where the ‘amine’ characteristic group was not recognized.

Examples:

$$\overset{7}{Sn}H_3\text{-}\overset{6}{O}\text{-}\overset{5}{Sn}H_2\text{-}\overset{4}{O}\text{-}\overset{3}{Sn}H_2\text{-}\overset{2}{O}\text{-}\overset{1}{Sn}H_3$$

tetrastannoxane (preselected name, see P-12.2)
$SiH_3\text{-}S\text{-}SiH_3$
disilathiane (preselected name, see P-12.2)
HS-O-SH
dithioxane (preselected name, see P-12.2)
$PH_2\text{-}Se\text{-}PH_2$
diphosphaselenane (preselected name, see P-12.2)
$SiH_3\text{-}NH\text{-}SiH_3$
N-silylsilanamine (name derived from the preselected name silane, see P-12.2)
(not disilazane)

P-21.2.3.2 Heterogeneous parent hydrides formed by skeletal replacement (‘a’) nomenclature

Heterogeneous acyclic parent hydrides consisting of chains containing at least one carbon atom and heteroatoms, alike or different, and terminating with C, P, As, Sb, Bi, Si, Ge, Sn, Pb, B, Al, Ga, In, or Tl are named by skeletal replacement (‘a’) nomenclature (see P-15.4.3). The use of skeletal replacement (‘a’) names as preferred IUPAC names is considered in Chapter P-5.

Examples:

11 10 9 8 7 6 5 4 3 2 1
$\mathrm{CH_3\text{-}O\text{-}CH_2\text{-}CH_2\text{-}O\text{-}CH_2\text{-}CH_2\text{-}O\text{-}CH_2\text{-}O\text{-}CH_3}$
2,4,7,10-tetraoxaundecane (PIN)

11 10 9 8 7 6 5 4 3 2 1
$\mathrm{CH_3\text{-}O\text{-}CH_2\text{-}CH_2\text{-}O\text{-}CH_2\text{-}CH_2\text{-}SiH_2\text{-}CH_2\text{-}S\text{-}CH_3}$
7,10-dioxa-2-thia-4-silaundecane (PIN)

8 7 6 5 4 3 2 1
$\mathrm{CH_3\text{-}S\text{-}SiH_2\text{-}CH_2\text{-}CH_2\text{-}SiH_2\text{-}O\text{-}CH_3}$
2-oxa-7-thia-3,6-disilaoctane (PIN)

P-21.2.4 Acyclic parent hydrides containing heteroatoms with nonstandard bonding numbers.

P-21.2.4.1 Heteroatoms with nonstandard bonding numbers are denoted by the λ^n symbol which is placed after each appropriate locant (see P-14.1). Low numbering is first given to the heteroatoms in the usual manner without regard to nonstandard bonding numbers. When there is a choice, lower locants are given to a higher nonstandard bonding number.

Examples:

1 2 3
$\mathrm{HS\text{-}SH_2\text{-}SH}$
$2\lambda^4$-trisulfane (preselected name, see P-12.2)

3 2 1
$\mathrm{HS\text{-}S\text{-}SH_5}$
$1\lambda^6$-trisulfane (preselected name, see P-12.2)

1 2 3
$\mathrm{PH_4\text{-}PH_3\text{-}PH_4}$
$1\lambda^5,2\lambda^5,3\lambda^5$-triphosphane (preselected name, see P-12.2)
(not tri-λ^5-phosphane)

1 2 3
$\mathrm{PH_4\text{-}O\text{-}PH_4}$
$1\lambda^5,3\lambda^5$-diphosphoxane (preselected name, see P-12.2)

P-21.2.4.2 When a choice is needed between the same skeletal atom with two or more nonstandard bonding numbers, low locants are assigned in order of the decreasing value of the bonding number, for example λ^6 is assigned a lower locant than λ^4.

Examples:

6 5 4 3 2 1
$\mathrm{HS\text{-}SH_2\text{-}S\text{-}S\text{-}SH_4\text{-}SH}$
$2\lambda^6,5\lambda^4$-hexasulfane (preselected name; see P-12.2)

12 11 10 9 8 7 6 5 4 3 2 1
$\mathrm{CH_3\text{-}S\text{-}CH_2\text{-}CH_2\text{-}SH_2\text{-}CH_2\text{-}CH_2\text{-}SH_4\text{-}CH_2\text{-}CH_2\text{-}S\text{-}CH_3}$
$2,5\lambda^6,8\lambda^4,11$-tetrathiadodecane (PIN)

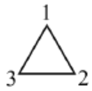
P-22 MONOCYCLIC PARENT HYDRIDES

P-22.1 Monocyclic hydrocarbons
P-22.2 Heteromonocyclic parent hydrides

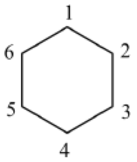
P-22.1 MONOCYCLIC HYDROCARBONS

P-22.1.1 The names of saturated monocyclic hydrocarbons are formed by attaching the nondetachable prefix ‘cyclo’ to the name of the acyclic saturated unbranched hydrocarbon with the same number of carbon atoms. The generic name of monocyclic hydrocarbons is ‘cycloalkane’. Numbering proceeds sequentially around the ring, usually clockwise. For unsaturated monocyclic hydrocarbons, see P-31.1.

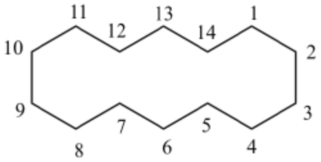
Examples:



cyclopropane (PIN)



cyclohexane (PIN)



cyclotetradecane (PIN)

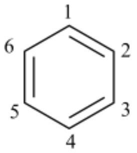
P-22.1.2 Unsubstituted monocyclic hydrocarbon polyenes having the maximum number of non-cumulative double bonds (mancude) and with the general formula of C_nH_n or C_nH_{n+1} (with *n* greater than 6) are called annulenes generically. A specific annulene is named as an [*n*]annulene, where *n* is the number of carbon atoms of the ring and is greater than 6. When *n* is an odd number, i. e., when the annulene has the general formula C_nH_{n+1}, the extra hydrogen atom is denoted as 'indicated hydrogen' (see P-14.7) and is assigned the locant '1'. Such annulene names may be used in general nomenclature and are the IUPAC preferred names for parent components in fusion nomenclature (P-25.3.2.1.1); but not as component prefixes.

Preferred IUPAC names for fully unsaturated monocyclic hydrocarbons are those of the corresponding cycloalkapolyenes (see P-31.1.3.1).

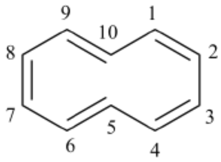
Benzene is the retained name for C_6H_6; the name [6]annulene is not recommended.

In the numbering of annulenes, the locant '1' is placed at any carbon atom in structures having an even number of carbon atoms; in annulenes having an odd number of carbon atoms, the locant '1' is assigned to the carbon atom bearing the indicated hydrogen (see P-14.7). In cycloalkapolyene structures, the locant '1' is always assigned to a carbon atom of a double bond.

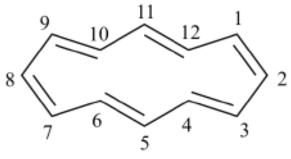
Examples:



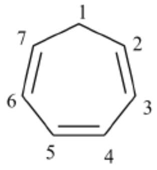
benzene (PIN; retained name)
(not [6]annulene)



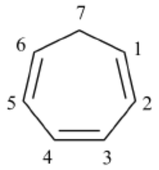
[10]annulene
cyclodeca-1,3,5,7,9-pentaene (PIN, P-25.3.2.1.1)



[12]annulene
cyclododeca-1,3,5,7,9,11-hexaene (PIN, P-31.1.3.1)

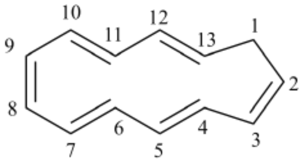


(**I**)

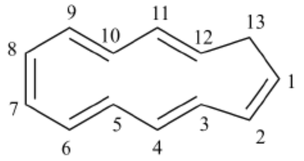


(**II**)

(**I**) 1*H*-[7]annulene
(**II**) cyclohepta-1,3,5-triene (PIN, P-31.1.3.1)



(**I**)



(**II**)

(**I**) 1*H*-[13]annulene
(**II**) cyclotrideca-1,3,5,7,9,11-hexaene (PIN, P-31.1.3.1)

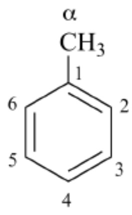
P-22.1.3 Parent hydrocarbons having retained names

Toluene, xylene, and mesitylene are specific parent hydrides that are composed of two components, one cyclic and the other acyclic and saturated. These names are retained due to a long and well established tradition. Toluene and xylene are preferred IUPAC names, but are not freely substitutable; toluene is substitutable under certain conditions, but only for general nomenclature (see P-15.1.8 for a general substitution rules for retained names).

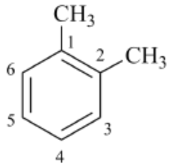
Mesitylene is a retained name in general nomenclature only and cannot be substituted.

The names cumene and cymene are not retained.

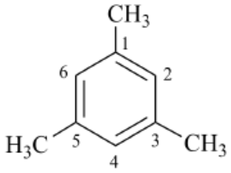
In the 1993 Guide (ref. 2) these parent hydrides were retained but only limited substitution was allowed.



toluene (PIN)
(no substitution; for general nomenclature
substitution is permitted only by groups listed in P-15.1.8.2.2)



xylene (1,2-, 1,3-, and 1,4-isomers, PINs)
(no substitution)
o-, *m*-, and *p*-xylene



mesitylene (no substitution)
1,3,5-trimethylbenzene (PIN)

P-22.2 HETEROMONOCYCLIC PARENT HYDRIDES

P-22.2.1 Retained names of heteromonocycles
P-22.2.2 Heteromonocyclic parent hydrides with 3-10 membered rings (Hantzsch-Widman names)
P-22.2.3 Heteromonocyclic parent hydrides named by skeletal replacement ('a') nomenclature
P-22.2.4 Heteromonocycles with eleven or more members with the maximum number of noncumulative double bonds
P-22.2.5 Homogeneous monocyclic parent hydrides other than boron hydrides
P-22.2.6 Heteromonocyclic parent hydrides composed of repeating heterounits
P-22.2.7 Heteromonocyclic parent hydrides having heteroatoms with nonstandard bonding numbers

P-22.2.1 Retained names of heteromonocycles

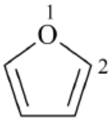
Retained names for 'mancude' heteromonocycles and their chalcogen analogues are listed in Table 2.2.

Note: The term 'mancude' is an acronym for MAximum number of NonCUmulative DoublE bonds.

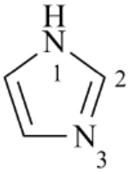
The name 'pyran' is modified by functional replacement nomenclature to generate names for chalcogen analogues.

Retained names for saturated heteromonocycles are given in Table 2.3.

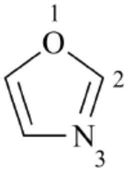
Table 2.2 Retained names of mancude heteromonocyclic parent hydrides

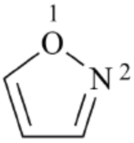


furan (PIN)

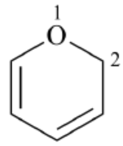


imidazole (1*H*-isomer shown;
the PIN is 1*H*-imidazole)

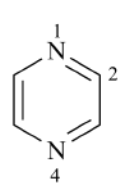




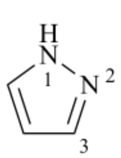
oxazole	isoxazole
1,3-oxazole (PIN)	1,2-oxazole (PIN)
thiazole (S instead of O)	isothiazole (S instead of O)
1,3-thiazole (PIN)	1,2-thiazole (PIN)
selenazole (Se instead of O)	isoselenazole (Se instead of O)
1,3-selenazole (PIN)	1,2-selenazole (PIN)
tellurazole (Te instead of O)	isotellurazole (Te instead of O)
1,3-tellurazole (PIN)	1,2-tellurazole (PIN)



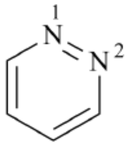
pyran (2*H*-isomer shown;
the PIN is 2*H*-pyran)
thiopyran (S instead of O) (2*H*-isomer shown;
the PIN is 2*H*-thiopyran)
selenopyran (Se instead of O) (2*H*-isomer shown;
the PIN is 2*H*-selenopyran)
telluropyran (Te instead of O) (2*H*-isomer shown;
the PIN is 2*H*-telluropyran)



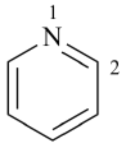
pyrazine (PIN)



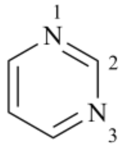
pyrazole (1*H*-isomer shown;
the PIN is 1*H*-pyrazole)



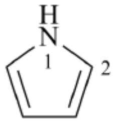
pyridazine (PIN)



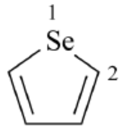
pyridine (PIN)



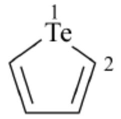
pyrimidine (PIN)



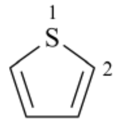
pyrrole (1*H*-isomer shown;
the PIN is 1*H*-pyrrole)



selenophene (PIN)

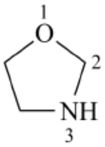


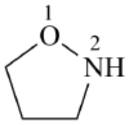
tellurophene (PIN)



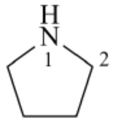
thiophene (PIN)

Table 2.3 Retained names of saturated heteromonocyclic parent hydrides

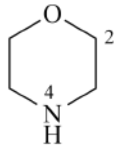




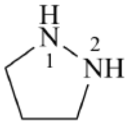
oxazolidine	isoxazolidine
1,3-oxazolidine (PIN)	1,2-oxazolidine (PIN)
thiazolidine (S instead of O)	isothiazolidine (S instead of O)
1,3-thiazolidine (PIN)	1,2-thiazolidine (PIN)
selenazolidine (Se instead of O)	isoselenazolidine (Se instead of O)
1,3-selenazolidine (PIN)	1,2-selenazolidine (PIN)
tellurazolidine (Te instead of O)	isotellurazolidine (Te instead of O)
1,3-tellurazolidine (PIN)	1,2-tellurazolidine (PIN)

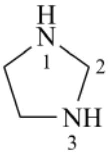


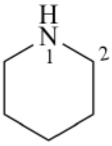
pyrrolidine (PIN)

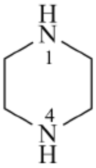


morpholine (PIN)
thiomorpholine (S instead of O) (PIN)
selenomorpholine (Se instead of O) (PIN)
telluromorpholine (Te instead of O) (PIN)


pyrazolidine (PIN)


imidazolidine (PIN)


piperidine (PIN)


piperazine (PIN)

P-22.2.2 Heteromonocyclic parent hydrides with 3 through 10 membered rings (Hantzsch-Widman names)

Heteromonocyclic parent hydrides with no more than ten ring members and containing one or more heteroatoms are named by using the extended Hantzsch-Widman system (ref. 21), a modification of the method published in the 1979 recommendations (ref. 1) that removes the need for many of the explanatory footnotes and comments. Homogeneous heteromonocyclic ring names are preselected (see P-12.2). The recommendations in the 1979 recommendations continue to be used in CAS fused ring names.

The elements aluminium, gallium, indium, and thallium are now included in the recommended Hantzsch-Widman system and mercury has been deleted.

P-22.2.2.1 Constructing and numbering Hantzsch-Widman names

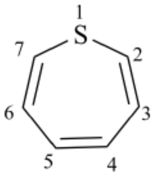
P-22.2.2.1.1 Hantzsch-Widman names are formed by combining skeletal replacement (‘a’) prefix(es) for the heteroatom(s) (Table 2.4) with a stem indicating the size of the ring and the degree of hydrogenation (Table 2.5). The final ‘a’ vowel between ‘a’ prefixes and between the ‘a’ prefix and the stem are elided. Unsaturated compounds are those having the maximum number of noncumulative double bonds (mancude compounds) and at least one double bond. The presence of a single heteroatom determines the numbering in a monocyclic compound; the heteroatom has the locant ‘1’ and the numbering usually proceeds clockwise, when unsubstituted.

Hantzsch-Widman names, except for azine and oxine, are preferred IUPAC names for both the unsaturated and saturated compounds. Azine must not be used for pyridine because of its long-established use as a class name for =N-N= compounds (see P-68.3.1.2.3). Oxine must not be used for pyran because it has been used as a trivial name for quinolin-8-ol.

Hantzsch-Widman names are preselected names for homogeneous heteromonocycles other than hydrocarbons (see P-22.2.5).

The final ‘e’ in Hantzsch-Widman names is required in preferred IUPAC names; it is still optional in general nomenclature. In the 1979 Rules (ref. 1), the final ‘e’ of a Hantzsch-Widman name was omitted when there was no nitrogen in the ring; in the 1993 Guide (ref. 2) this omission was made optional.

Examples:


thiepine (PIN)

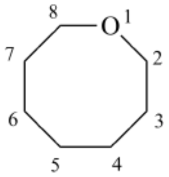

oxocane (PIN)

Table 2.4 Hantzsch-Widman system prefixes (in decreasing order of seniority)

Element	Bonding Number (Valence)	Prefix	Element	Bonding Number (Valence)	Prefix
fluorine	1	fluora	antimony	3	stiba
chlorine	1	chlora	bismuth	3	bisma
bromine	1	broma	silicon	4	sila
iodine	1	ioda	germanium	4	germa
oxygen	2	oxa	tin	4	stanna
sulfur	2	thia	lead	4	plumba
selenium	2	selena	boron	3	bora
tellurium	2	tellura	aluminium	3	aluma[1] (not alumina)
nitrogen	3	aza	gallium	3	galla
phosphorus	3	phospha	indium	3	indiga[1] (not inda)
arsenic	3	arsa	thallium	3	thalla

[1] Compare with Table 1.5

Table 2.5 Hantzsch-Widman system stems

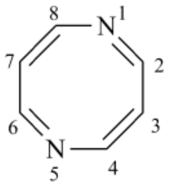
Ring Size	Unsaturated	Saturated	Ring Size	Unsaturated	Saturated
3	irene/irine[1]	irane/iridine[2]	7	epine	epane
4	ete	etane/etidine[2]	8	ocine	ocane
5	ole	olane/olidine[2]	9	onine	onane
6A (O, S ,Se, Te, Bi)	ine	ane	10	ecine	ecane
6B (N, Si, Ge, Sn, Pb)	ine	inane			
6C (F, Cl, Br, I, P, As, Sb, B, Al, Ga, In, Tl)	inine	inane			

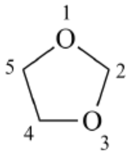
[1] See P-22.2.2.1.5.1

[2] See P-22.2.2.1.5.2

P-22.2.2.1.2 A multiplicity of the same heteroatom is indicated by a multiplying prefix 'di', 'tri', 'tetra', etc., placed before the appropriate 'a' term. The final letter 'a' of a multiplying prefix is elided before a vowel, e.g., tetrazole, not tetraazole. Lowest possible locants are assigned to heteroatoms, locant '1' being assigned to one of the heteroatoms. Locants are cited at the front of the name, i.e., before the skeletal replacement ('a') term and any preceding numerical prefixes.

Examples:

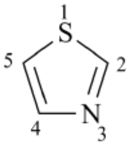

1,5-diazocine (PIN)



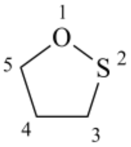
1,3-dioxolane (PIN)

P-22.2.2.1.3 If two or more kinds of heteroatoms occur in the same name, their order of citation follows the sequence: F, Cl, Br, I, O, S, Se, Te, N, P, As, Sb, Bi, Si, Ge, Sn, Pb, B, Al, Ga, In, Tl. The locant '1' is given to a heteroatom that occurs first in the seniority sequence used for citation of the skeletal replacement ('a') prefixes. The numbering is then chosen to give lowest locants to heteroatoms considered as a set in ascending numerical order. Locants are cited at the front of the name, in the order of citation of the skeletal replacement ('a') prefixes.

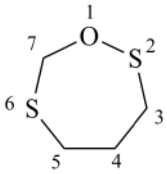
Examples:



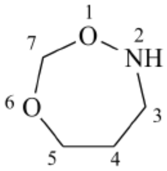
1,3-thiazole (PIN)



1,2-oxathiolane (PIN)



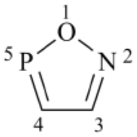
1,2,6-oxadithiepane (PIN)
(not 1,3,7-oxadithiepane;
the locant set '1,2,6' is lower than '1,3,7')



1,6,2-dioxazepane (PIN)
(not 1,3,4-dioxazepane;
not 1,3,7-dioxazepane;
not 1,6,5-dioxazepane;
the locant set '1,2,6' is lower than '1,3,4', '1,3,7', or '1,5,6')

If there is a further choice, lowest locants are assigned to heteroatoms in the order that they appear in the seniority sequence (see Table 2.4).

Example:

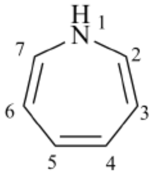


1,2,5-oxazaphosphole (PIN)
(not 1,5,2-oxazaphosphole;
N has priority over P for lowest locant)

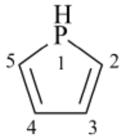
P-22.2.2.1.4 Indicated hydrogen

After the maximum number of noncumulative double bonds has been assigned to the ring structure, any ring atom with a bonding number of three or higher connected to adjacent ring atoms by single bonds only, and carrying one or more hydrogen atoms, is designated by indicated hydrogen (see P-14.7). If there is a choice, such ring atoms are assigned low locants.

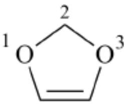
Examples:



1*H*-azepine (PIN)



1*H*-phosphole (PIN)



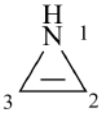
2*H*-1,3-dioxole (PIN)

P-22.2.2.1.5 Selecting Hantzsch-Widman names for 3-, 4-, or 5-membered rings

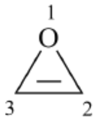
As shown in Table 2.5, for mancude three-membered rings and saturated three-, four-, and five-membered rings two stems are recommended. They are used as follows to generate preferred IUPAC names:

P-22.2.2.1.5.1 The stem 'irine' is used in place of 'irene' for rings only containing nitrogen heteroatoms; otherwise the stem 'irene' is used.

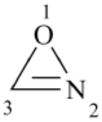
Examples:



1*H*-azirine (PIN)



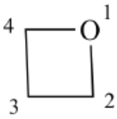
oxirene (PIN)



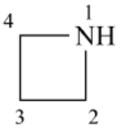
oxazirene (PIN)

P-22.2.2.1.5.2 The stems 'iridine', 'etidine', and 'olidine' are used when nitrogen atoms are present in the ring; otherwise the 'ane' stems are used.

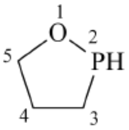
Examples:



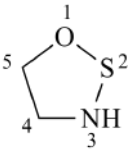
oxetane (PIN)



azetidine (PIN)



1,2-oxaphospholane (PIN)

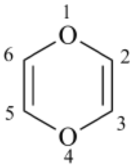


1,2,3-oxathiazolidine (PIN)

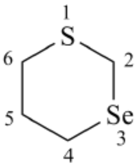
P-22.2.2.1.6 Selecting Hantzsch-Widman names for six-membered rings

The stem for six-membered rings depends on the least senior heteroatom in the ring, i.e., the heteroatom whose name directly precedes the stem. Heteroatoms are divided into three groups, A, B, and C, each corresponding to a stem for the unsaturated and for the saturated compound (Table 2.5). The stem is selected in accordance with the group to which the least senior heteroatom belongs.

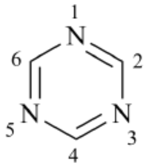
Examples:



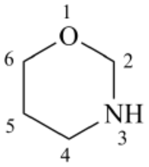
1,4-dioxine (PIN)



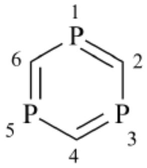
1,3-thiaselenane (PIN)



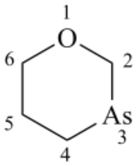
1,3,5-triazine (PIN)



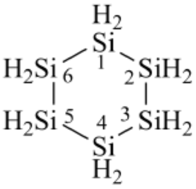
1,3-oxazinane (PIN)



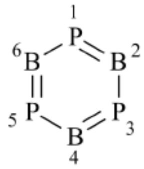
1,3,5-triphosphinine (PIN)

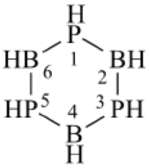


1,3-oxarsinane (PIN)



hexasilinane (preselected name; see P-12.2)

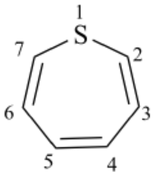

1,3,5,2,4,6-triphosphatriborinine
(preselected name; see P-12.2)

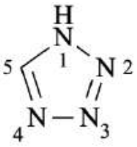

1,3,5,2,4,6-triphosphatriborinane (preselected name; see P-12.2)

P-22.2.2.1.7 Omission of locants

All locants are omitted for parent Hantzsch-Widman names if there is only one heteroatom or if there is no ambiguity if locants are omitted.

Examples:


thiepine
(not 1-thiepine)

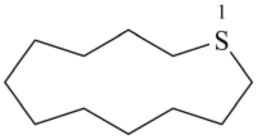

1*H*-tetrazole
(not 1*H*-1,2,3,4-tetrazole)

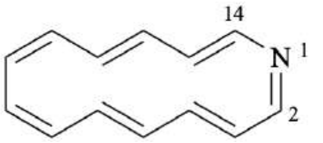
P-22.2.3 Heteromonocyclic hydrides named by skeletal replacement (‘a’) nomenclature

Mancude and saturated heteromonocyclic compounds with up to and including ten ring members are named by the extended Hantzsch-Widman system (see P-22.2.2). For monocyclic rings with eleven and more ring members, skeletal replacement (‘a’) nomenclature (see P-15.4) is used for the fully saturated or fully unsaturated compounds ([*n*]annulenes).

P-22.2.3.1 Skeletal replacement (‘a’) names are formed by placing skeletal replacement (‘a’) prefixes (see Table 2.4) in front of the name of the corresponding cycloalkane or annulene, and, when more than one heteroatom is present, in the following decreasing seniority order: F > Cl > Br > I > O > S > Se > Te > N > P > As > Sb > Bi > Si > Ge > Sn > Pb > B > Al > Ga > In > Tl. For numbering, see P-22.2.3.2. The selection of preferred IUPAC names is discussed in P-52.2.3.

Examples:


thiacyclododecane (PIN)

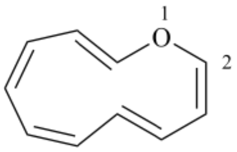

1-azacyclotetradeca-1,3,5,7,9,11,13-heptaene (PIN)
aza[14]annulene

P-22.2.3.2 Numbering

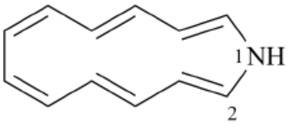
P-22.2.3.2.1 When a single heteroatom is present in the ring, it is assigned the locant ‘1’, which is omitted in the name, unless a locant for an indicated hydrogen atom is present. Numbering usually proceeds clockwise, unless substituted.

Low locants are assigned first to the heteroatom and then to unsaturated sites (see P-31.1.3.2). When required, locants for indicated hydrogen atoms are assigned in accordance with P-14.7

Examples:



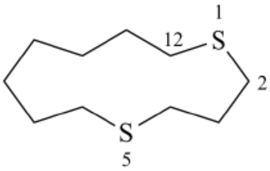
1-oxacycloundeca-2,4,6,8,10-pentaene (PIN)
oxa[11]annulene



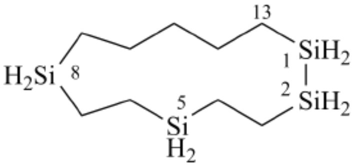
1-azacyclotrideca-2,4,6,8,10,12-hexaene (PIN)
1*H*-1-aza[13]annulene

P-22.2.3.2.2 When the same kind of heteroatom occurs more than once, the direction of numbering is chosen to give the lower locants to the heteroatoms as a set.

Examples:



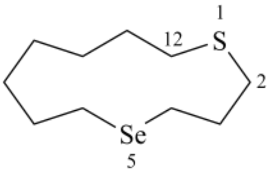
1,5-dithiacyclododecane (PIN)
(not 1,9-dithiacyclododecane)



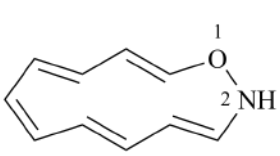
1,2,5,8-tetrasilacyclotridecane (PIN)
(other locant sets are: ‘1,2,8,11’, ‘1,4,7,8’, ‘1,4,5,11’, and ‘1,4,10,11’,
none of which are lower than ‘1,2,5,8’)

P-22.2.3.2.3 When heteroatoms of different kinds are present, the locant ‘1’ is given to the heteroatom first cited in the order of seniority given above (see P-22.2.3.1). The direction of numbering is then chosen to give lower locants to the heteroatoms as a set without regard to the kind of heteroatom, and then, if necessary, according to the order of seniority above (see P-22.2.3.1). Low locants are assigned first to the heteroatoms and then to unsaturated sites (see P-31.1.3.2). When required, locants for indicated hydrogen atoms are assigned in accordance with P-14.7.

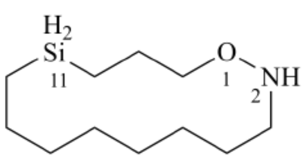
Examples:



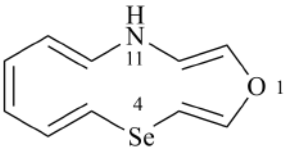
1-thia-5-selenacyclododecane (PIN)



1-oxa-2-azacyclododeca-3,5,7,9,11-pentaene (PIN)
2*H*-1-oxa-2-aza[12]annulene



1-oxa-2-aza-11-silacyclotetradecane (PIN)



1-oxa-4-selena-11-azacyclotrideca-2,5,7,9,12-pentaene (PIN)
11*H*-1-oxa-4-selena-11-aza[13]annulene

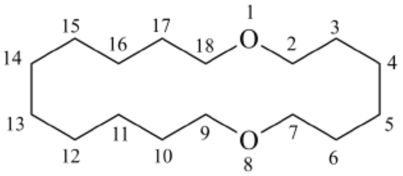
P-22.2.4 Heteromonocycles with eleven or more members with the maximum number of noncumulative double bonds.

Names of heteromonocyclic parent components with more than ten ring members are discussed in this subsection. They are used to generate names of preferred IUPAC names of fused ring systems; they have also been used as names for the heteromonocycle in general nomenclature as an alternative to cycloalkapolyene names that are preferred IUPAC names for the heteromonocycles.

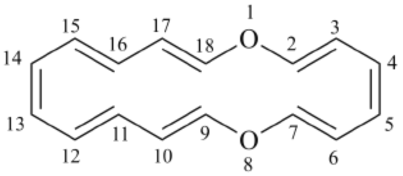
A heteromonocyclic parent component having more than ten ring members and the maximum number of noncumulative double bonds (mancude) is named by changing the ending 'ane' of the name corresponding to the saturated heteromonocycle (see P-22.2.3) to 'ine'. Locants are cited at the front of the name, in the order of citation of the corresponding skeletal replacement ('a') prefixes. Indicated hydrogen atoms are designated as required. In organometallic nomenclature, a modified skeletal replacement ('a') nomenclature is allowed in smaller rings to create metallacycle parent hydrides (see P-69.4).

For examples of fusion compounds including this type of heteromonocyclic component, see P-25.2.2.4, P-25.3.6.1 and P-25.3.7.1.

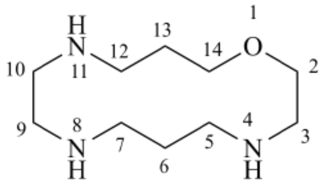
Examples:



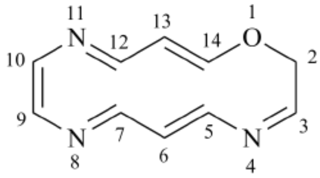
1,8-dioxacyclooctadecane (PIN)



1,8-dioxacyclooctadecine
1,8-dioxacyclooctadeca-2,4,6,9,11,13,15,17-octaene (PIN)



1-oxa-4,8,11-triazacyclotetradecane (PIN)

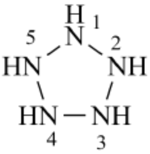


2*H*-1,4,8,11-oxatriazacyclotetradecine
1-oxa-4,8,11-triazacyclotetradeca-3,5,7,9,11,13-hexaene (PIN)

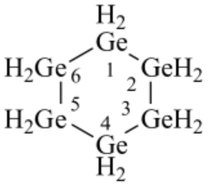
P-22.2.5 Homogeneous heteromonocyclic parent hydrides other than boron hydrides.

A saturated heteromonocycle consisting of identical heteroatoms can be named by adding the prefix 'cyclo' to the name of the saturated unbranched chain that has the same number of identical atoms. For alternative methods, see the Hantzsch-Widman extended system described in P-22.2.2 for rings with 3 through 10 members and skeletal replacement ('a') nomenclature described in P-22.2.3. For the names that are preselected (see P-12.2) but used to generate preferred IUPAC names for organic derivatives, see P-52.1.5.

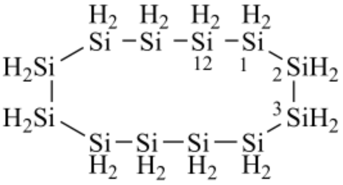
Examples:



cyclopentaazane
pentazolidine
(preselected name; see P-22.2.2.1.5)



cyclohexagermane
hexagerminane
(preselected name; see P-12.2)

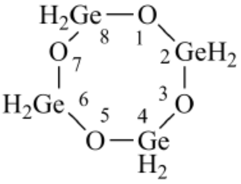


cyclododecasilane
dodecasilacyclododecane
(preselected name; see P-12.2)

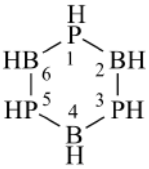
P-22.2.6 Heteromonocyclic parent hydrides composed of repeating units [(ab)$_n$ cyclic hydrides].

Names may be constructed by citing successively the prefix 'cyclo', a multiplying affix ('di', 'tri', 'tetra', etc.) indicating the number of each element in the ring, the skeletal replacement ('a') terms for the atoms of the repeated unit first cited in the order Tl > In > Ga > Al > Pb > Sn > Ge > Si > Bi > Sb> As > P > N > Te > Se > S> O, and the ending 'ane'. The terminal letter of a skeletal replacement ('a') term is elided when followed by a vowel; the terminal letter of a multiplying affix is not elided even when the 'a' term begins with a vowel. Numbering starts at one of the skeletal atoms of the element cited last in the name and proceeds continuously around the ring. For alternative methods, see P-22.2.2 for Hantzsch-Widman names and P-22.2.3 for monocycles with more than ten ring members. For the preselected names (see P-12.2) used to generate the preferred IUPAC names for organic derivatives of these heteromonocyclic hydrides, see P-52.1.5.2.

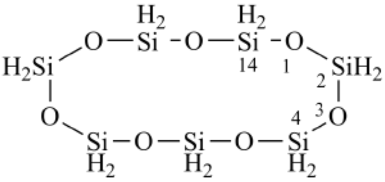
Examples:



cyclotetragermoxane
1,3,5,7,2,4,6,8-tetroxatetragermocane
(preselected name, see P-12.2)



cyclotriboraphosphane
1,3,5,2,4,6-triphosphatriborinane
(preselected name, see P-12.2)



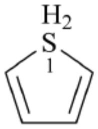
cycloheptasiloxane

1,3,5,7,9,11,13-heptaoxa-2,4,6,8,10,12,14-heptasilacyclotetradecane
(preselected name, see P-12.2, P-22.2.3.2.3)

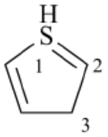
P-22.2.7 Heteromonocyclic hydrides having heteroatoms with nonstandard bonding numbers.

P-22.2.7.1 The λ-convention is used to denote heteroatoms with nonstandard bonding numbers in heteromonocycles (see P-14.1). The symbol λ^n, where *n* is the bonding number, is cited immediately after the locant denoting the heteroatom with the nonstandard bonding number. The indicated hydrogen symbol *H*, if required to denote saturated skeletal atoms, is cited at the front of the complete name with the appropriate locant(s).

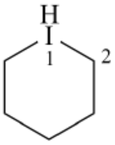
Examples:



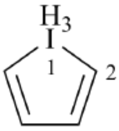
1*H*-1λ^4-thiophene (PIN)



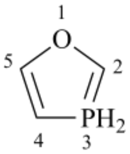
3*H*-1λ^4-thiophene (PIN)



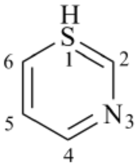
1λ^3-iodinane (PIN)



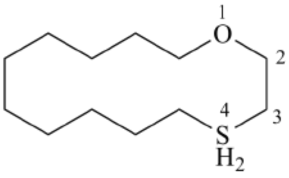
1*H*-1λ^5-iodole (PIN)



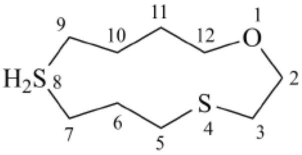
1,3λ^5-oxaphosphole (PIN)



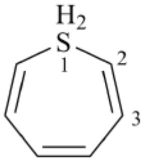
1λ^4,3-thiazine (PIN)



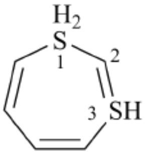
1-oxa-4λ^4-thiacyclotetradecane (PIN)



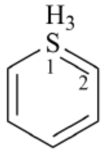
1-oxa-4,8λ^4-dithiacyclododecane (PIN)



1H-1λ^4-thiepine (PIN)



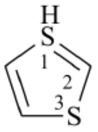
1H-1λ^4,3λ^4-dithiepine (PIN)
[the (–SH_2–) group, which includes an indicated hydrogen, is preferred for the lowest locant]



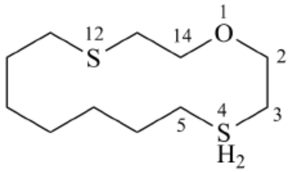
1λ^6-thiopyran (PIN)
(this heteromonocycle has the maximum number of double bonds and one double bond at every position;
hence, no indicated hydrogen is cited for the sulfur atom)

P-22.2.7.2 If a further choice is needed between two or more of the same skeletal atom with different bonding numbers, the lower locant is assigned in order of the decreasing value of the bonding number, i.e., λ^6 is selected over λ^4 (see also P-21.2.4).

Examples:



1λ^4,3-dithiole (PIN)



1-oxa-4λ^4,12-dithiacyclotetradecane (PIN)

P-23 POLYALICYCLIC PARENT HYDRIDES (Extended von Baeyer System)

P-23.0 Introduction
P-23.1 Definitions and terminology
P-23.2 Naming and numbering of von Baeyer hydrocarbons
P-23.3 Heterogeneous heterocyclic von Baeyer parent hydrides
P-23.4 Homogeneous heterocyclic von Baeyer parent hydrides
P-23.5 Heterogeneous heterocyclic von Baeyer parent hydrides composed of alternating heteroatoms
P-23.6 Heterocyclic polyalicyclic parent hydrides having heteroatoms with nonstandard bonding numbers
P-23.7 Retained names for von Baeyer parent hydrides

P-23.0 INTRODUCTION

This section is based on the recent publication “Extension and Revision of the von Baeyer system for naming polycyclic compounds (including bicyclic compounds) (IUPAC Recommendations 1999)” (ref. 7). It supersedes Rules A-31, A-32, and B-14 in the 1979 Recommendations (ref. 1) and Rule R-2.4.2 in the 1993 Recommendations (ref. 2). No modifications to the 1999 publication have been made in this Section.

This Section deals only with saturated polyalicyclic ring systems named by the von Baeyer system; for unsaturated systems, see Section P-31.1.4. For naming substituent groups derived from saturated polyalicyclic ring systems, see Section P-29.

P-23.1 DEFINITIONS AND TERMINOLOGY

P-23.1.1 A ‘bridgehead’ is any skeletal atom of the ring system that is bonded to three or more skeletal atoms (excluding hydrogen).

P-23.1.2 A ‘bridge’ is an unbranched chain of atoms or an atom or a valence bond connecting two bridgeheads.

P-23.1.3 The ‘main ring’ is the ring system that includes as many skeletal atoms of the polycyclic system as possible.

P-23.1.4 The ‘main bridge’ is the bridge included in a bicyclic system and the first selected bridge in a polycyclic system.

P-23.1.5 Two bridgeheads are selected as ‘main bridgeheads’. These two bridgeheads are included in the main ring and connected by the main bridge.

P-23.1.6 A ‘secondary bridge’ is any bridge not included in the main ring or the main bridge.

P-23.1.7 An ‘independent secondary bridge’ links bridgeheads which are part of the main ring or main bridge.

P-23.1.8 A ‘dependent secondary bridge’ links at least one bridgehead that is part of a secondary bridge.

P-23.1.9 A ‘polycyclic system’ contains a number of rings equal to the minimum number of scissions required to convert the system into an acyclic skeleton. The number of rings is indicated by the nondetachable prefix ‘bicyclo’ (not dicyclo), ‘tricyclo’, ‘tetracyclo’, etc.

P-23.2 NAMING AND NUMBERING OF VON BAEYER HYDROCARBONS

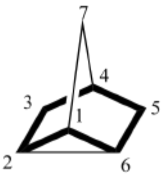
Bi- and polycyclic hydrocarbons that are treated by the von Baeyer system are named by the following rules applied in order until a decision is reached.

P-23.2.1 Selection of the main ring
P-23.2.2 Naming bicyclic alicyclic hydrocarbons
P-23.2.3 Numbering bicyclic alicyclic hydrocarbons
P-23.2.4 Selection of the main bridge
P-23.2.5 Naming and numbering tricyclic alicyclic hydrocarbons
P-23.2.6 Naming and numbering polyalicyclic hydrocarbons

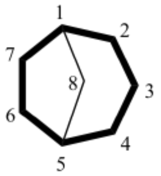
P-23.2.1 Selection of the main ring

The main ring of a polycyclic hydrocarbon ring system is selected so as to include as many skeletal atoms of the structure as possible. The main ring is shown as bold lines in subsections P-23.2.1 through P-23.2.6.

Examples:



a six-membered main ring

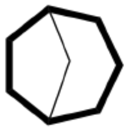


a seven-membered main ring

P-23.2.2 Naming bicyclic alicyclic hydrocarbons

Saturated homogeneous bicyclic hydrocarbons having two or more atoms in common are named by prefixing ‘bicyclo’ to the name of the acyclic hydrocarbon having the same total number of skeletal atoms. The numbers of skeletal atoms in each of the two segments connecting the main bridgeheads and in the main bridge are given by arabic numbers cited in descending numerical order, separated by full stops, and enclosed in square brackets.

Example:

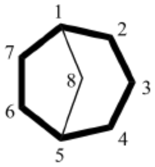


bicyclo[3.2.1]octane (PIN)

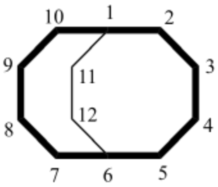
P-23.2.3 Numbering bicyclic alicyclic hydrocarbons

The bicyclic ring system is numbered starting with one of the bridgeheads and proceeding first along the longer segment of the main ring to the second bridgehead, then back to the first bridgehead along the unnumbered segment of the main ring. Numbering is completed by numbering the main bridge beginning with the atom next to the first bridgehead.

Examples:



bicyclo[3.2.1]octane (PIN)

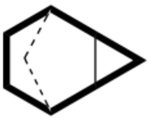


bicyclo[4.4.2]dodecane (PIN)

P-23.2.4 Selection of the main bridge

In a polycyclic ring system there is more than one bridge connecting atoms of the main ring and/or the main bridge. In the tricyclic ring below, the main ring is shown in solid bold lines, and the main bridge, shown in the dashed lines, is the bridge that includes as many of the atoms as possible that are not included in the main ring. Bridges other than the main bridge are called ‘secondary bridges’, appearing below as a normal solid line.

Example:



P-23.2.5 Naming and numbering tricyclic alicyclic hydrocarbons

P-23.2.5.1 Tricyclic hydrocarbons having an independent secondary bridge are named on the basis of a bicyclic system described in P-23.2.2. Rings not described by the bicyclic system are defined by citing the number of atoms in the independent secondary bridge as an arabic number. The locants of the two attachment points of the independent secondary bridge to the main ring are cited as a pair of superscript arabic numbers (lower number is cited first) separated by a comma.

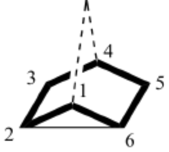
The name of the tricyclic system is then constructed by citing:

(a) the prefix ‘tricyclo’, in place of ‘bicyclo’, indicating the presence of three rings in the polyalicyclic system;

(b) numbers indicating the bridge lengths, starting with the two branches of the main ring (shown as a bold line in the structures below), followed by the main bridge (shown in dotted bold lines in the structures below), and the secondary bridge (with superscript locants separated by commas indicating its points of attachment to the main ring), all separated by full stops and placed in brackets, for example [2.2.1.0^{2,6}];

(c) the name of the acyclic hydrocarbon having the same total number of skeletal atoms.

Example:

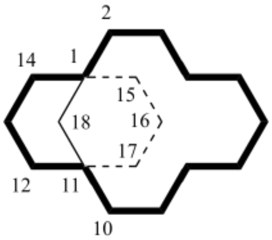


tricyclo[2.2.1.0^{2,6}]heptane (PIN)

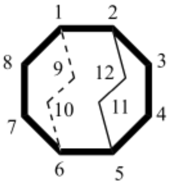
P-23.2.5.2 Numbering the secondary bridge

After the main ring and main bridge have been numbered, the independent secondary bridge is numbered continuing from the higher numbered bridgehead of the main ring.

Examples:



tricyclo[9.3.3.$1^{1,11}$]octadecane (PIN)



tricyclo[4.2.2.$2^{2,5}$]dodecane (PIN)
[the secondary bridge is numbered starting from bridgehead 5,
the higher (than 2) numbered bridgehead]

P-23.2.6 Naming and numbering polycyclic alicyclic hydrocarbons

Polycyclic analogues of saturated bi- and tricyclic ring systems (P-23.2.3 and P-23.2.5) are named as described in the following subsections. Independent and dependent secondary bridges are considered here. Rules for numbering all secondary bridges and for naming all polyalicyclic systems are described; their application follows those described for naming and numbering bicyclic systems as described in P-23.2.1 through P-23.2.4 above. An additional rule is necessary to select the main bridge and the secondary bridges.

P-23.2.6.1 Naming polycyclic alicyclic hydrocarbons

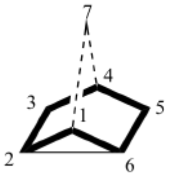
Rings not designated by the bicyclic system described above (P-23.2.2) are defined by citing the number of atoms in each secondary bridge as an arabic number. The locants of the two attachment points of each secondary bridge to the main ring are cited as a pair of superscript arabic numbers (lower first) separated by a comma. The numbers indicating independent secondary bridges (bridges that connect atoms of the bicyclic system) are cited in decreasing order. The procedure for construction of names is given in the following subsections.

P-23.2.6.1.1 The prefixes ‘tricyclo’, ‘tetracyclo’, etc., in place of vbicyclo’, indicate the number of rings in the polyalicyclic system. The number of rings is equal to the number of bond cuts necessary to transform the polycyclic system into an acyclic skeleton, unbranched or branched.

P-23.2.6.1.2 The number of atoms in each bridge additional to the main bridge, i.e., the secondary bridges, is indicated by arabic numbers separated by full stops and cited in decreasing numerical order following those describing the bicyclic system, except as provided by P-23.2.6.1.3. The location of each secondary bridge is indicated by the arabic number locants of the bicyclic structure already numbered; these locants are cited as superscripts to the arabic number denoting its length (number of atoms) and separated by a comma. The assemblage of arabic numbers denoting the length of bridges with superscript numbers, if necessary, is commonly called the ‘von Baeyer descriptor’ and is enclosed in brackets.

P-23.2.6.1.3 Independent secondary bridges are cited before dependent secondary bridges. The numbers indicating dependent secondary bridges are cited in decreasing order (the third example in P-23.2.6.3 illustrates this order of citation).

P-23.2.6.1.4 The name is terminated by the name of the alkane representing the total number of ring atoms; this number corresponds to the sum of the arabic numbers in the numerical descriptor enclosed by brackets plus two (for the two main bridgehead atoms); for example, in the name ‘bicyclo[2.2.1.$0^{2,6}$]heptane’ for the following structure, the total number of ring atoms, 7, equals the sum of the primary numbers in the descriptor, [2 + 2 + 1+ 0], + 2.



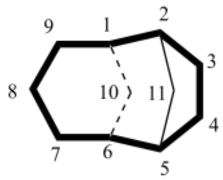
P-23.2.6.2 Selection of the main bridge and secondary bridges

There are often a number of choices to be made in the selection of the main bridge and the secondary bridges. To make such choices, the following criteria are applied in order until a decision can be made.

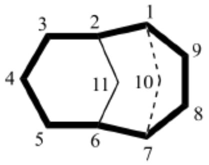
Note: Numberings shown in the examples below follow the rules given in P-23.2.6.3.

P-23.2.6.2.1 The main ring must be divided as symmetrically as possible by the main bridge, which, as directed in P-23.2.4, includes as many of the atoms not included in the main ring as possible.

Example:


9
1
2
3
8
10
11
4
7
6
5

not


3
2
1
9
4
11
10
8
5
6
7

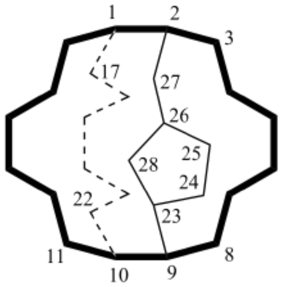
tricyclo[4.3.1.1^{2,5}]undecane (PIN)
correct

tricyclo[5.2.1.1^{2,6}]undecane
incorrect

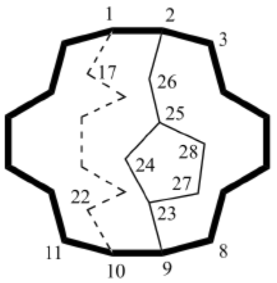
Explanation: Two bridges of 4 and 3 atoms divide the main ring more symmetrically than two bridges of 5 and 2 atoms.

P-23.2.6.2.2 If there is a choice for independent secondary bridges, the first cited must be as long as possible. Then, if relevant, the second must be as long as possible, etc.

Example:


1
2
3
17
27
26
25
28
24
22
23
11
8
10
9

not


1
2
3
17
26
25
28
24
27
22
23
11
8
10
9

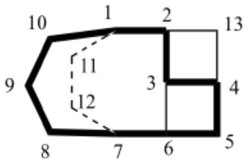
tetracyclo[8.6.6.5^{2,9}.1^{23,26}]octacosane (PIN)
correct

tetracyclo[8.6.6.4^{2,9}.2^{23,25}]octacosane
incorrect

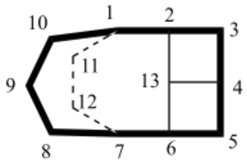
Explanation: The five-atom independent bridge between positions 2 and 9 of the main ring is longer than the four-atom independent bridge between positions 2 and 9.

P-23.2.6.2.3 The number of dependent secondary bridges is to be kept to a minimum.

Example:


10
1
2
13
11
9
3
4
12
8
7
6
5

not


10
1
2
3
11
13
9
4
12
8
7
6
5

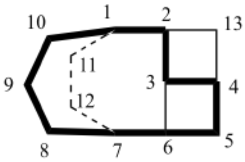
tetracyclo[5.3.2.1^{2,4}.0^{3,6}]tridecane (PIN)
correct

tetracyclo[5.3.2.1^{2,4}.0^{6,13}]tridecane
incorrect

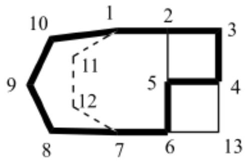
Explanation: There are no dependent bridges in the correct structure; there is dependent bridge in the incorrect structure, between 6 and 13.

P-23.2.6.2.4 The superscript locants for the secondary bridges must be as low as possible when considered as a set in ascending numerical order, the decision being made at the first point of difference.

Examples:


10
1
2
13
11
9
3
4
12
8
7
6
5

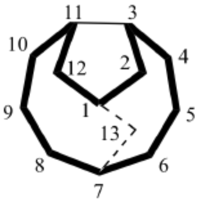
not


10
1
2
3
11
9
5
4
12
8
7
6
13

tetracyclo[5.3.2.1^{2,4}.0^{3,6}]tridecane (PIN)
correct

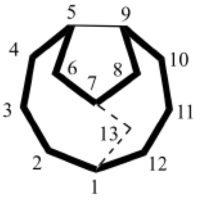
tetracyclo[5.3.2.1^{4,6}.0^{2,5}]tridecane
incorrect

Explanation: The locant set ‘2,3,4,6’ is lower than ‘2,4,5,6’; see P-14.3.5.


11
3
10
12
2
4
9
1
5
13
8
6
7

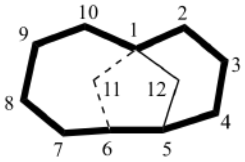
tricyclo[5.5.1.$0^{3,11}$]tridecane
correct

not


5
9
4
6
7
8
10
3
11
13
2
12
1

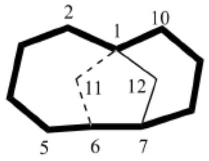
tricyclo[5.5.1.$0^{5,9}$]tridecane
incorrect

Explanation: The locant set '3,11' is lower than '5,9'; see P-14.3.5.


10
2
9
1
3
11
12
8
4
7
6
5

tricyclo[4.4.1.$1^{1,5}$]dodecane (PIN)
correct

not

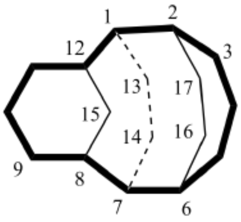

2
1
10
11
12
5
6
7

tricyclo[4.4.1.$1^{1,7}$]dodecane
incorrect

Explanation: The locant set '1,5' is lower than '1,7'; see P-14.3.5.

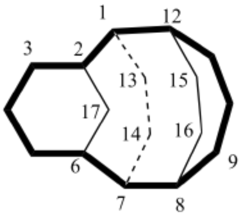
P-23.2.6.2.5 The superscript locants shall be as low as possible when considered in the sequence of their order of citation in the name.

Examples:


1
2
12
3
13
17
15
14
16
9
8
7
6

tetracyclo[5.5.2.$2^{2,6}$.$1^{8,12}$]heptadecane (PIN)
correct

not


1
12
3
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13
15
17
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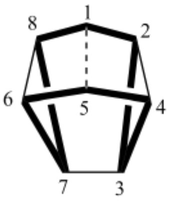
16
9
6
7
8

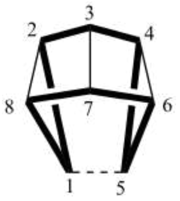
tetracyclo[5.5.2.$2^{8,12}$.$1^{2,6}$]heptadecane
incorrect

Explanation: The locant sequence '2,6,8,12' is lower than '8,12,2,6'; see P-14.3.5.



pentacyclo[3.3.0.$0^{2,4}$.$0^{3,7}$.$0^{6,8}$]octane (PIN)
correct

not



pentacyclo[3.3.0.$0^{2,8}$.$0^{3,7}$.$0^{4,6}$]octane
incorrect

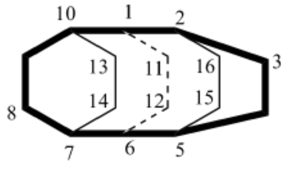
Explanation: The locant sequence '2,4,3,7,6,8' is lower than '2,8,3,7,4,6'; see P-14.3.5

P-23.2.6.3 Numbering of secondary bridges

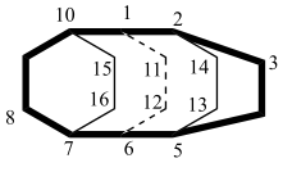
After numbering the main ring and main bridge, independent secondary bridges are numbered before dependent secondary bridges; the numbering continues from the highest number of the main ring and main bridge. Each secondary bridge is numbered in turn starting with the independent secondary bridge linked to the highest numbered bridgehead atom of the main ring, then the independent secondary bridge linked to the next highest bridgehead atom, and so on. Each atom of a secondary bridge is numbered starting with the atom next to the higher numbered bridgehead.

Note: Rule A-32.23 in the 1979 Recommendations (ref. 1) and Rule R-2.4.2.2 in the l993 Recommendations (ref. 2) have been replaced by this Rule.

Examples:


10
1
2
13
11
16
3
14
12
15
8
7
6
5

not


10
1
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11
14
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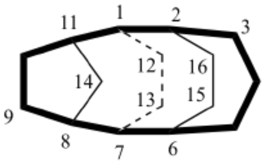
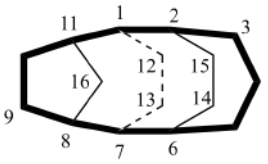
16
12
13
8
7
6
5

tetracyclo[4.4.2.2^{2,5}.2^{7,10}]hexadecane (PIN)

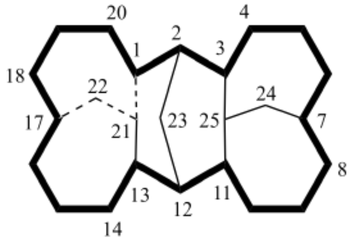
Explanation: The first secondary bridge to be numbered is linked to bridgehead 10.


11
1
2
3
12
16
14
13
15
9
8
7
6

not


11
1
2
3
12
15
16
13
14
9
8
7
6

tetracyclo[5.4.2.2^{2,6}.1^{8,11}hexadecane (PIN)
(the first secondary bridged to be numbered is linked to bridgehead 11)


20
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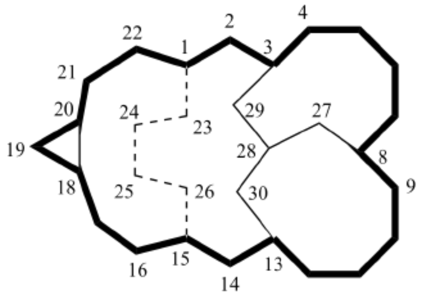
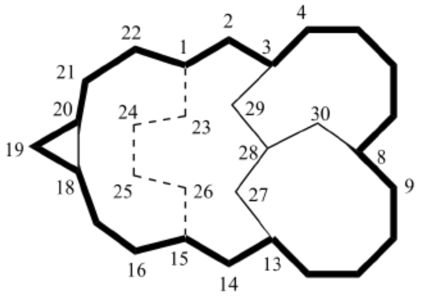
2
1
3
18
22
24
17
21
23
25
7
8
13
11
12
14

hexacyclo[15.3.2.2^{3,7}.1^{2,12}.0^{13,21}.0^{11,25}]pentacosane
(the dependent secondary bridge between atoms numbered 11 and 25 is cited last;
in the numeric descriptor, the numbers ‘15, 3, and 2’ describe the basic bicyclic system;
the numbers 2^{3,7},1^{2,12}, and 0^{13,21} correspond to the three independent secondary bridges;
the number 0^{11,25} corresponds to the dependent secondary bridge)
octadecahydro-6,13-methano-2,14:7,9-dipropanodicyclohepta[*a*,*e*][8]annulene (PIN)
(see P-25.4.3.4.2)
[not octadecahydro-7,14-methano-4,6:8,10-dipropanodicyclohepta[*a*,*d*][8]annulene;
in the correct name a greater number of rings of the fusion ring system to be bridged are in a horizontal row,
3 versus 2; see P-25.3.2.3.3 (a) and P-44.2.2.2.3 (b)]


22
2
4
1
3
21
20
24
29
27
23
19
28
8
18
25
26
30
9
16
15
13
14

not


22
2
4
1
3
21
20
24
29
30
23
19
28
8
18
25
26
27
9
16
15
13
14

(I)
correct

(II)
incorrect

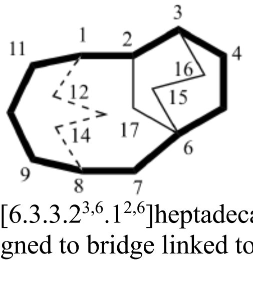
(I) pentacyclo[13.7.4.3^{3,8}.0^{18,20}.1^{13,28}]triacontane (PIN)
(II) pentacyclo[13.7.4.3^{3,13}.0^{18,20}.1^{8,28}]triacontane

Explanation: In the correct name **(I)**, the PIN, the independent bridge is numbered before the dependent bridge; locant sequence ‘3,8,18,20,13,28’ is lower than ‘3,13,18,20,8,28’ (see P-14.3.5).

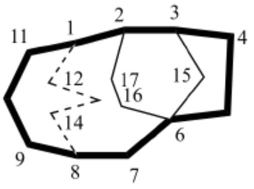
P-23.2.6.4 If there is a further choice for numbering the secondary bridges, the following criteria are considered in order until a decision can be made.

P-23.2.6.4.1 Lower locants are used for the atoms of the bridge linked to the higher numbered bridgehead.

Examples:


3
11
1
2
4
16
12
15
17
14
6
9
8
7

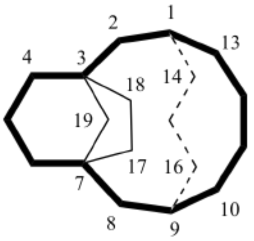
tetracyclo[6.3.3.2^{3,6}.1^{2,6}]heptadecane (PIN)
(locants 15 and 16 are assigned to bridge linked to bridgehead atom 3 not 2)



tetracyclo[6.3.3.2^{2,6}.1^{3,6}]heptadecane (PIN)
(the locant 15 is assigned to the bridge linked to bridgehead atom 3 not 2)

P-23.2.6.4.2 Longer bridges are numbered before shorter bridges.

Example:

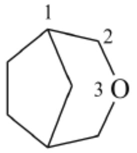


tetracyclo[7.4.3.2^{3,7}.1^{3,7}]nonadecane (PIN)
(the two-atom bridge between bridgehead atoms 3 and 7 is numbered before
the one-atom bridge between the same two bridgehead atoms).

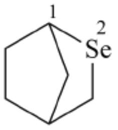
P-23.3 HETEROGENEOUS HETEROCYCLIC VON BAEYER PARENT HYDRIDES

P-23.3.1 The only general method to name heterogeneous heterocyclic von Baeyer systems is skeletal replacement (‘a’) nomenclature. The replacement (‘a’) prefixes denoting the heteroatoms are placed in front of the name of the corresponding hydrocarbon named according to P-23.2, cited in the order: F > Cl > Br > I > O > S > Se > Te > N > P > As > Sb > Bi >Si > Ge > Sn > Pb > B > Al > Ga > In > Tl. Numbering is determined first by the fixed numbering of the hydrocarbon system.

Examples:



3-oxabicyclo[3.2.1]octane (PIN)

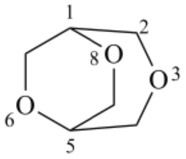


2-selenabicyclo[2.2.1]heptane (PIN)

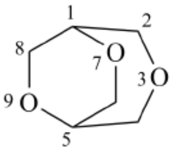
P-23.3.2 When there is a choice for numbering, the following criteria are applied in order until a decision can be made.

P-23.3.2.1 Low locants are assigned to the heteroatoms considered together as a set compared in increasing numerical order. The preferred numbering is the lowest set at the first point of difference.

Example:



not



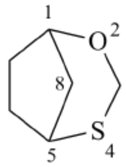
3,6,8-trioxabicyclo[3.2.2]nonane (PIN)
correct

3,7,9-trioxabicyclo[3.2.2]nonane
incorrect

Explanation: The locant set ‘3,6,8’ is lower than ‘3,7,9’ (see P-14.3.5)

P-23.3.2.2 If there is still a choice, low locants are assigned in accord with the decreasing seniority order of heteroatoms O > S > Se > Te > N > P > As > Sb > Bi > Si > Ge > Sn > Pb > B > Al > Ga > In > Tl.

Example:



2-oxa-4-thiabicyclo[3.2.1]octane (PIN)

P-23.4 HOMOGENEOUS HETEROCYCLIC VON BAEYER PARENT HYDRIDES

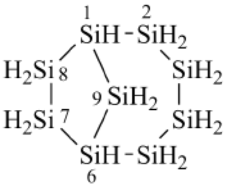
Heterocyclic von Baeyer systems composed entirely of the same heteroatom are named:

(a) as described for bi- and polycyclic hydrocarbons in P-23.2 using the name of the acyclic parent hydride that has the same total number of skeletal atoms; or

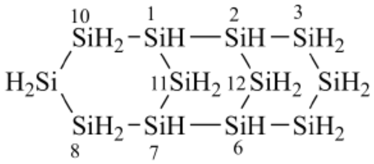
(b) by skeletal replacement nomenclature using the replacement (‘a’) prefixes described in P-22.2.5, in which the total number of heteroatoms is indicated by a numerical term.

In either method it is not necessary to give the location of the heteroatoms because all positions are modified by the same heteroatom. For the preselected names (see P-12.2) that are used to generate PIN names for organic derivatives see P-52.1.5.

Examples:



(a) bicyclo[4.2.1]nonasilane (preselected name; see P-12.2)
(b) nonasilabicyclo[4.2.1]nonane



(a) tricyclo[5.3.1.1^{2,6}]dodecasilane (preselected name; see P-12.2)
(b) dodecasilatricyclo[5.3.1.1^{2,6}]dodecane

P-23.5 HETEROGENEOUS HETEROCYCLIC VON BAEYER PARENT HYDRIDES COMPOSED OF ALTERNATING HETEROATOMS

P-23.5.1 Heterogeneous von Baeyer systems composed of alternating skeletal heteroatoms may be named in two ways:

(a) by citing a nondetachable prefix ‘bicyclo’, ‘tricyclo’, etc. before a von Baeyer descriptor (see P-23.2.2, P-23.2.5, and P-23.2.6) enclosed in square brackets and then, successively:

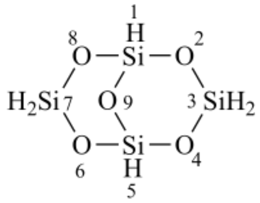
- (i) a multiplying prefix, ‘di’, ‘tri’, etc., denoting the number of heteroatoms that are first cited as replacement (‘a’) terms;
- (ii) the sketetal replacement (‘a’) terms denoting the heteroatoms of the system in the reverse order of the recommended seniority for ‘a’ prefixes (for example, Si before O; see P-23.3.1);
- (iii) the ending ‘ane’.

Numbering is the same as for the corresponding hydrocarbon (see P-23.2.3 and P-23.2.6.3);

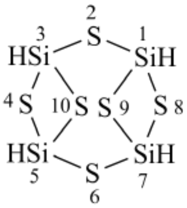
(b) by applying normal skeletal replacement (‘a’) nomenclature to the corresponding hydrocarbon.

For the preselected names (see P-12.2) that are used to generate PIN names for organic derivatives see P-52.1.6.2.

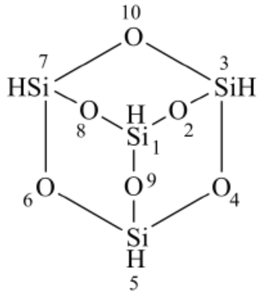
Examples:



(a) bicyclo[3.3.1]tetrasiloxane (preselected name; see P-12.2)
(b) 2,4,6,8,9-pentaoxa-1,3,5,7-tetrasilabicyclo[3.3.1]nonane



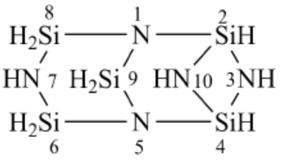
(a) tricyclo[5.1.1.$1^{3,5}$]tetrasilathiane (preselected name; see P-12.2)
(b) 2,4,6,8,9,10-hexathia-1,3,5,7-tetrasilatricyclo[5.1.1.$1^{3,5}$]decane



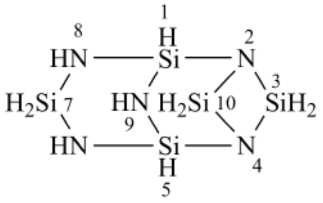
(a) tricyclo[3.3.1.$1^{3,7}$]tetrasiloxane (preselected name; see P-12.2)
(b) 2,4,6,8,9,10-hexaoxa-1,3,5,7-tetrasilatricyclo[3.3.1.$1^{3,7}$]decane

P-23.5.2 The prefixes '*Si*-' or '*N*-' preceded by the italic number '1' are used when necessary to specify the atom at the bridgehead that is to have the locant '1'. Names are identified as (a) and (b) according to the two methods described in P-23.5.1.

Examples:



(a) *1N*-tricyclo[3.3.1.$1^{2,4}$]pentasilazane (preselected name; see P-12.2)
(b) 1,3,5,7,10-pentaaza-2,4,6,8,9-pentasilatricyclo[3.3.1.$1^{2,4}$]decane

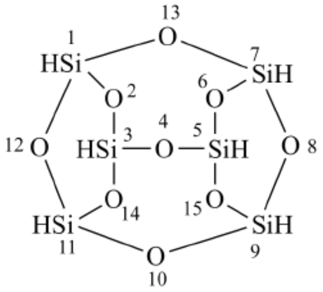


(a) *1Si*-tricyclo[3.3.1.$1^{2,4}$]pentasilazane (preselected name; see P-12.2)
(b) 2,4,6,8,9-pentaaza-1,3,5,7,10-pentasilatricyclo[3.3.1.$1^{2,4}$]decane

P-23.5.3 Silasesquioxanes, silasesquithianes, etc.

Compounds in which each silicon atom is linked to three oxygen atoms and in which every atom of oxygen is linked to two silicon atoms are named generically silasesquioxanes. Similarly, when the oxygen atoms are replaced by S, Se, Te, or N atoms, the compounds are generically called silasesquithianes, silasesquiazanes, and so forth. They are named by the method described in P-23.5.1 (a). Silasesquioxanes have the general formula $Si_{2n}H_{2n}O_{3n}$. The names tetrasilasesquioxanes ($n = 2$), hexasilasesquioxanes ($n = 3$), etc., are class names indicating $Si_{2n}H_{2n}E_{3n}$ where E = O; and similarly when E = S, Se, Te, or N. Silasesquiazanes have the general formula $Si_{2n}H_{5n}N_{3n}$.

Example:

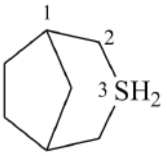


tetracyclo[5.5.1.1^{3,11}.1^{5,9}]hexasiloxane (a hexasilasesquioxane)
(preselected name; see P-12.2)
2,4,6,8,10,12,13,14,15-nonaoxa-1,3,5,7,9,11-hexasilatetracyclo[5.5.1.1^{3,11}.1^{5,9}]pentadecane

P-23.6 HETEROCYCLIC POLYALICYCLIC PARENT HYDRIDES HAVING HETEROATOMS WITH NONSTANDARD BONDING NUMBERS

P-23.6.1 The λ-convention, characterized by the symbol λ^n, where '*n*' is the bonding number of the heteroatom, is used to identify heteroatoms with nonstandard bonding numbers (see P-14.1). The symbol is placed before the appropriate 'a' prefix.

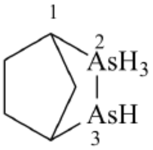
Example:



3λ^4-thiabicyclo[3.2.1]octane (PIN)

P-23.6.2 When there is a choice for numbering, low locants are assigned to heteroatoms with nonstandard bonding numbers expressed by the λ^n symbol in order of decreasing numerical value of the bonding number; for example, in the case of arsenic, the lower locant is given to a λ^5 arsenic atom.

Example:

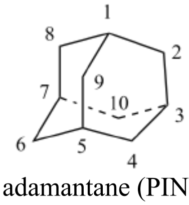


2λ^5,3-diarsabicyclo[2.2.1]heptane (PIN)

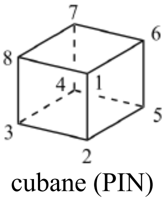
P-23.7 RETAINED NAMES FOR VON BAEYER PARENT HYDRIDES

The retained names adamantane and cubane are used in general nomenclature and as preferred IUPAC names. The name quinuclidine is retained for general nomenclature only (see Table 2.6). The name prismane is no longer recommended.

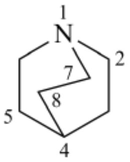
Table 2.6 Retained names for von Baeyer parent hydrides



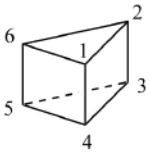
adamantane (PIN)
tricyclo[3.3.1.1^{3,7}]decane



cubane (PIN)
pentacyclo[4.2.0.0^{2,5}.0^{3,8}.0^{4,7}]octane



quinuclidine
1-azabicyclo[2.2.2]octane (PIN)



tetracyclo[2.2.0.0^{2,6}.0^{3,5}]hexane (PIN)
(not prismane)

P-24 SPIRO RING SYSTEMS

P-24.0 Introduction
P-24.1 Definitions
P-24.2 Spiro ring systems with only monocyclic ring components
P-24.3 Monospiro ring systems containing two identical polycyclic ring components
P-24.4 Three identical polycyclic ring components spirofused together
P-24.5 Monospiro ring systems with different ring components at least one of which is a polycyclic ring system
P-24.6 Unbranched polyspiro ring systems with different ring components, one being a polycyclic ring system
P-24.7 Branched polyspiro ring systems
P-24.8 Spiro ring systems containing atoms with nonstandard bonding numbers

P-24.0 INTRODUCTION

This Section is based on the recent publication ‘Extension and Revision of the Nomenclature for Spiro Compounds, IUPAC Recommendations1999’ (ref. 8). It supersedes Rules A-41, A-43, B-10, and B-12 in the 1979 Recommendations (ref. 1) and Rule R-2.4.3 in the 1993 Recommendations (ref. 2). The alternative methods given by Rules A-42 and B-11 in the 1979 recommendations (ref. 1) have been abandoned.

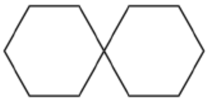
Section P-24.5.2 takes into account appropriate modifications to Section SP-4.1 of the 1999 publication (ref. 8). Also in P-24.5.3, P-24.6, P-24.7 and P-24.8.4 some modifications on the usage of brackets have been made to SP-4, SP-5 and SP-7 of the 1999 publication (ref. 8).

The spiro ring systems consisting only of monocyclic rings in this Section are saturated systems; for unsaturated systems, see Section P-31.1.5.1.

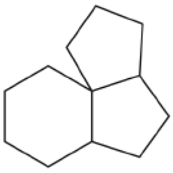
For naming substituent groups see Sections P-29 and P-32.1.3.

P-24.1 DEFINITIONS

A ‘spiro union’ is a linkage between two rings that consists of a single atom common to both rings. A ‘free spiro union’ is a linkage that constitutes the only direct union between the two rings.



a free spiro union



a non-free spiro union

The common atom is designated as the ‘spiro atom’. According to the number of spiro atoms present, compounds are distinguished as monospiro, dispiro, trispiro, etc., ring systems. The following recommendations apply only to the naming of parent hydrides containing free spiro unions. For naming spiro compounds with non-free spiro unions, see nomenclature of fused systems (see P-25 and ref. 8).

Spirofusion is the creation of one, and only one, common atom between two rings or ring systems, each ring or ring system contributing one, and only one, atom to the spiro ring system. It is analogous to the *ortho*- or *ortho*- and *peri*-fusion that creates common bonds between mancude rings or ring systems. Traditionally, *ortho*- or *ortho*- and *peri*-fusion has been called ‘fusion’, with no reference to its specific type of fusion. To avoid any ambiguity, the term ‘spiro’ must always be specified when added to the term ‘fusion’.

P-24.2 SPIRO RING SYSTEMS WITH ONLY MONOCYCLIC RING COMPONENTS

P-24.2.0 Introduction
P-24.2.1 Monospiro alicyclic ring systems
P-24.2.2 Linear polyspiro alicyclic ring systems
P-24.2.3 Branched polyspiro alicyclic ring systems
P-24.2.4 Heterocyclic spiro ring systems

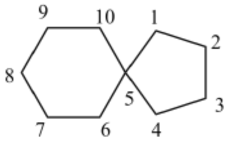
P-24.2.0 Introduction

This Section is concerned only with saturated spiro ring systems that consist only of monocyclic rings. For unsaturated alicyclic spiro ring systems, see Section P-31.1.5.

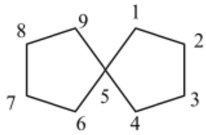
P-24.2.1 Monospiro alicyclic ring systems

Monospiro parent hydrides consisting of two saturated cycloalkane rings are named by placing the nondetachable prefix ‘spiro’ before the name of the unbranched acyclic hydrocarbon with the same total number of skeletal atoms. The number of skeletal atoms linked to the spiro atom in each ring is indicated by arabic numbers separated by a full stop, cited in ascending order and enclosed in square brackets; this descriptor (called in these recommendations the ‘von Baeyer spiro descriptor’) is placed between the spiro prefix and the name of the acyclic alkane. Numbering starts in the smaller ring, if one is smaller, at a ring atom next to the spiro atom and proceeds first around that ring, then through the spiro atom and around the second ring.

Examples:



spiro[4.5]decane (PIN)

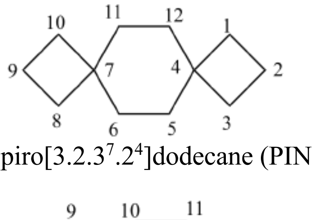


spiro[4.4]nonane (PIN)

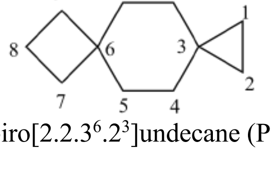
P-24.2.2 Linear polyspiro alicyclic ring systems

Polyspiro parent hydrides consisting of unbranched assemblies of three or more saturated cycloalkane rings are named using the nondetachable prefixes ‘dispiro’, ‘trispiro’, etc., according to the number of spiro atoms present, cited in front of the name of the acyclic hydrocarbon that has the same number of skeletal atoms. The von Baeyer spiro descriptor indicates the number of carbon atoms linking the spiro atoms by arabic numbers that are cited in order, starting at the smaller terminal ring if one is smaller, and proceeding consecutively, always by the shorter path, to the other terminal ring through each spiro atom and then back to the first spiro atom; the numbers are separated by full stops and enclosed in square brackets. The compound is numbered in the order in which the numbers of the von Baeyer spiro descriptor are cited, including spiro atoms when encountered for the first time. Each time a spiro atom is reached for the second time its locant, which has already been assigned, is cited as a superscript number to the number of the preceding linking atoms.

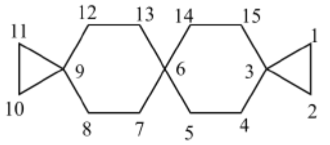
Examples:



dispiro[$3.2.3^7.2^4$]dodecane (PIN)



dispiro[$2.2.3^6.2^3$]undecane (PIN)

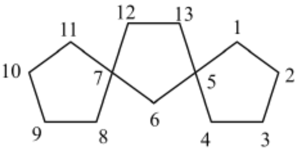


trispiro[$2.2.2.2^{9}.2^{6}.2^{3}$]pentadecane (PIN)

The use of superscript numbers was introduced in the publication 'Extension and Revision of the Nomenclature for Spiro Compounds and IUPAC Recommendations 1999' (ref. 8). Even though they are not needed in dispiro compounds, their use in branched spiro systems is essential for deriving unambiguous names; therefore, it is recommended that they be used to name all polyspiro compounds, especially when IUPAC preferred names are required.

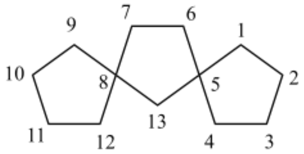
P-24.2.2.1 If there is a choice of numbers for the spiro descriptor, the smaller numbers are selected because low locants must be allocated to spiro atoms.

Examples:



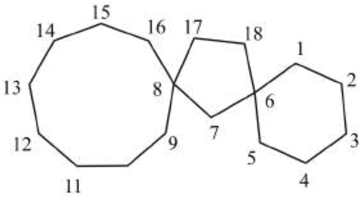
dispiro[$4.1.4^{7}.2^{5}$]tridecane (PIN)
correct

not



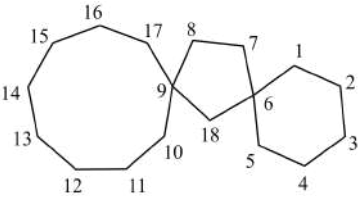
dispiro[$4.2.4^{8}.1^{5}$]tridecane
incorrect

Explanation: In the correct name, the number set '4,1' is lower than '4,2' and/or the spiro atom locant set 5,7 is smaller than 5,8.



dispiro[$5.1.8^{8}.2^{6}$]octadecane (PIN)
correct

not

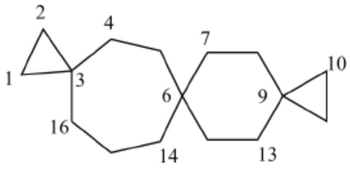


dispiro[$5.2.8^{9}.1^{6}$]octadecane
incorrect

Explanation: In the correct name, the number set '5,1' is lower than '5,2' and/or the spiro atom locant set 6,8 is smaller than 6,9.

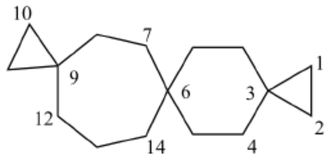
P-24.2.2.2 If there is still a choice of numbering, the numbers of the von Baeyer descriptors are considered in the sequence of the order of their citation. The name is selected with lower numbers at the first point of difference.

Example:



trispiro[$2.2.2.2^{9}.2^{6}.3^{3}$]hexadecane (PIN)
correct

not



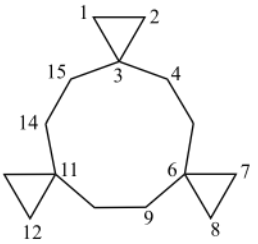
trispiro[$2.2.2.2^{9}.3^{6}.2^{3}$]hexadecane
incorrect

Explanation: In the correct name, the number set '$2,2,2,2^{9},2^{6},3^{3}$' is lower than '$2,2,2,2^{9},3^{6},2^{3}$'.

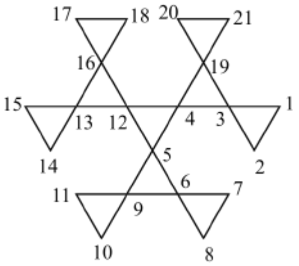
P-24.2.3 Branched polyspiro alicyclic ring systems

Branched polyspiro hydrocarbons composed only of cycloalkane rings are named using 'dispiro', 'trispiro', etc. before the name of the acyclic hydrocarbon corresponding to the total number of skeletal atoms present. The von Baeyer spiro descriptor indicates the number of skeletal atoms linking the spiro atoms by arabic numbers that are cited in order, starting at the smallest terminal ring, if one is smallest, proceeding consecutively to succeeding terminal rings through each spiro atom, always by the shortest path, and then back to the first spiro atom; the numbers are separated by full stops and enclosed in square brackets. The compound is numbered in the order in which the numbers of the spiro von Baeyer descriptor are cited, including spiro atoms when encountered for the first time. Each time a spiro atom is reached for the second time its locant is cited as a superscript number to the preceding number of linking atoms.

Examples:


1
2
15
3
4
14
11
6
7
12
9
8

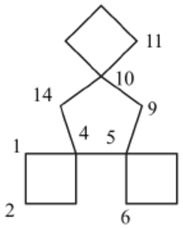
trispiro[2.2.2^{6}.2.2^{11}.2^{3}]pentadecane (PIN)
(the importance of superscripts is illustrated by this example and the third example in P-24.2.2;
without the superscripts these different compounds would have identical names)


17
18
20
21
16
19
15
1
13
12
4
3
14
5
2
6
7
11
9
10
8

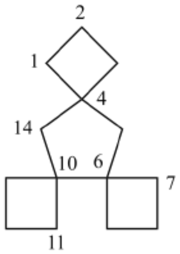
nonaspiro[2.0.0.0.2^{6}.0.2^{9}.0^{5}.0.0.2^{13}.0.2^{16}.0^{12}.0^{4}.0.2^{19}.0^{3}]henicosane (PIN)

P-24.2.3.1 If there is a choice for numbering, lowest locants are assigned to the spiro atoms.

Examples:


11
10
14
9
1
4
5
2
6

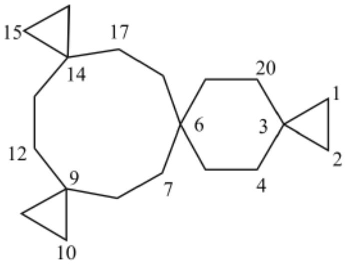
not


2
1
4
14
10
6
7
11

trispiro[3.0.3^{5}.1.3^{10}.1^{4}]tetradecane (PIN)
correct

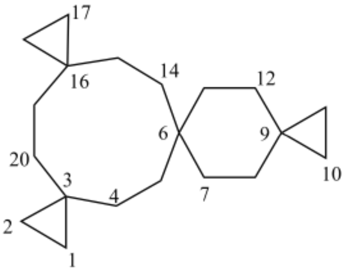
trispiro[3.1.3^{6}.0.3^{10}.1^{4}]tetradecane
incorrect

Explanation: In the correct name, the number set of the descriptor ‘3,0’ is lower than ‘3,1’ and/or the spiro atom locant set ‘4,5,10’ is lower than ‘4,6,10’.


15
17
14
20
1
6
3
12
9
2
7
4
10

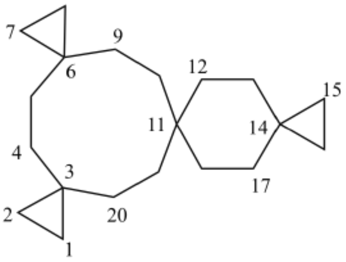
tetraspiro[2.2.2.2^{9}.2.2^{14}.2^{6}.2^{3}]icosane (PIN)
correct

not


17
14
16
12
6
9
20
3
4
10
2
7
1

tetraspiro[2.2.2.2^{9}.2^{6}.2.2^{16}.2^{3}]icosane
incorrect

not

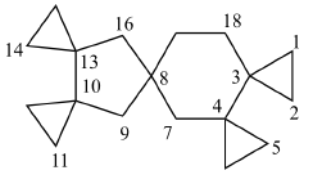

7
9
6
12
15
11
14
4
3
17
2
20
1

tetraspiro[2.2.2^{6}.2.2.2^{14}.2^{11}.2^{3}]icosane
incorrect

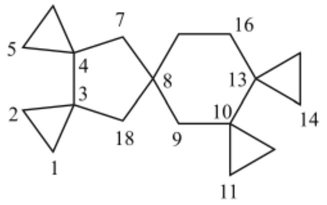
Explanation: In the correct name, the spiro locant set ‘3,6,9,14’ is lower than ‘3,6,9,16’ or ‘3,6,11,14’

P-24.2.3.2 If there is still a choice of numbering, the numbers of the von Baeyer descriptor are considered in their order of citation. The correct name has the lower numbers at first point of difference.

Example:



not



pentaspiro[2.0.2^{4}.1.1.2^{10}.0.2^{13}.1^{8}.2^{3}]octadecane (PIN)
correct

pentaspiro[2.0.2^{4}.1.1.2^{10}.0.2^{13}.2^{8}.1^{3}]octadecane
incorrect

Explanation: In the correct name, the PIN, the number sequence of the descriptor ‘2,0,2,1,1,2,0,2,1,2’ is lower than the number sequence ‘2,0,2,1,1,2,0,2,2,1’ for the incorrect name; at the ninth position, the number ‘1’ is lower than ‘2’

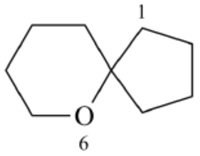
P-24.2.4 Heterocyclic spiro ring systems

P-24.2.4.1 Heterocyclic spiro ring systems named by skeletal replacement (‘a’) nomenclature
P-24.2.4.2 Homogeneous heterocyclic spiro ring systems with only monocyclic ring components
P-24.2.4.3 Heterocyclic spiro ring systems with only monocyclic ring components composed of alternating heteroatoms

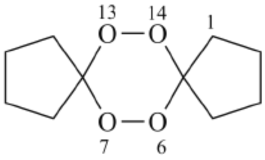
P-24.2.4.1 Heterocyclic spiro ring systems named by skeletal replacement (‘a’) nomenclature

P-24.2.4.1.1 When heteroatoms are present in a spiro ring system composed of only monocyclic rings, skeletal replacement (‘a’) nomenclature is used to name the heterocyclic system. The name of the corresponding hydrocarbon ring system is first constructed as described above (P-24.2.1, P-24.2.2, P-24.2.3). Heteroatoms are then introduced by using the general principles of skeletal replacement (‘a’) nomenclature. The numbering of the spiro hydrocarbon ring system is never modified by the introduction of heteroatoms, but low locants must be attributed to heteroatoms if there is a choice.

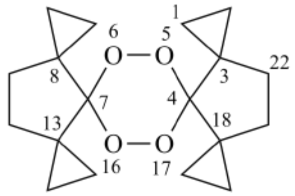
Examples:



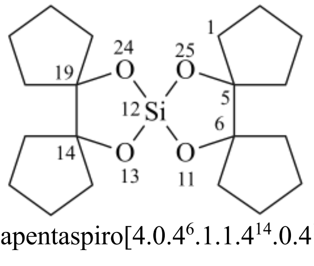
6-oxaspiro[4.5]decane (PIN)
(not 10-oxaspiro[4.5]decane)



6,7,13,14-tetraoxadispiro[4.2.4^{8}.2^{5}]tetradecane (PIN)



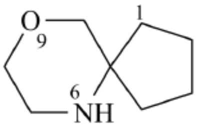
5,6,16,17-tetraoxahexaspiro[2.0.2.0.2^{8}.2.2^{13}.0^{7}.2^{4}.0.2^{18}.2^{3}]docosane (PIN)



11,13,24,25-tetraoxa-12-silapentaspiro[4.0.4^{6}.1.1.4^{14}.0.4^{19}.1^{12}.1^{5}]pentacosane (PIN)

P-24.2.4.1.2 If there is a choice of name or numbering due to heteroatoms, the following criteria are considered in order until a decision is reached:

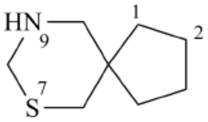
(a) low locants are allocated to heteroatoms as a set regardless of the kind of heteroatom;



9-oxa-6-azaspiro[4.5]decane (PIN)

(b) if there is still a choice, low locants are assigned in accord with the following decreasing seniority order of heteroatoms: F > Cl > Br > I > O > S > Se > Te > N > P > As > Sb > Bi > Si > Ge > Sn > Pb > B > Al > Ga > In > Tl.

Example:

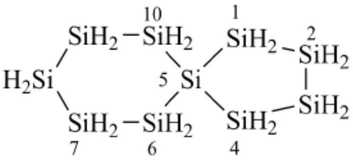


7-thia-9-azaspiro[4.5]decane (PIN)

P-24.2.4.2 Homogeneous heterocyclic spiro ring systems with only monocyclic ring components

Heterocyclic spiro ring systems with only monocyclic ring components and composed entirely of the same heteroatom are named as described above using the name of the homogeneous heteroacyclic ring system that has the same total number of skeletal heteroatoms. This method is preferred to skeletal replacement (‘a’) nomenclature described in P-24.2.4.1, in which the total number of heteroatoms is indicated by a numerical term. In either method it is not necessary to give the location of the heteroatoms because all positions are modified by the same heteroatom. For the preselected names (see P-12.2) that are used to generate PIN names for organic derivatives see P-52.1.6.

Example:



spiro[4.5]decasilane (preselected name; see P-12.2)
decasilaspiro[4.5]decane

P-24.2.4.3 Heterocyclic spiro ring systems with only monocyclic ring components composed of alternating heteroatoms

Heterocyclic spiro ring systems consisting only of monocyclic rings and having alternating skeletal heteroatoms are named by two methods.

(1) by citing a prefix such as ‘spiro’, ‘dispiro’, etc., before a von Baeyer descriptor (indicating the numbers of heteroatoms linked to each spiro atom in each ring cited in increasing order and separated by a full stop) enclosed in square brackets followed successively by:

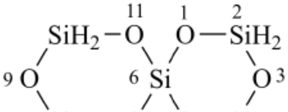
(a) a multiplying prefix (‘di’, ‘tri’, etc) denoting the number of heteroatoms of the first cited ‘a’ term that follows;

(b) the ‘a’ terms of the hetero atoms, cited in the reverse seniority order for ‘a’ prefixes (see P-21.2.3.1), for example, Si before O;

(c) the ending ‘ane’. The hetero spiro system is numbered as is the corresponding hydrocarbon.

(2) by skeletal replacement (‘a’) nomenclature as described in P-24.2.4.1.

For the preselected names (see P-12.2) that are used to generate PIN names for organic derivatives see P-52.1.6.2.

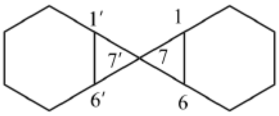


spiro[5.5]pentasiloxane (preselected name; see P-12.2)
1,3,5,7,9,11-hexaoxa-2,4,6,8,10-pentasilaspiro[5.5]undecane

P-24.3 MONOSPIRO RING SYSTEMS CONTAINING TWO IDENTICAL POLYCYCLIC COMPONENTS

P-24.3.1 Monospiro ring systems consisting of two identical polycyclic ring components are named by placing the nondetachable prefix ‘spirobi’ before the name of the component ring system enclosed in square brackets. The established numbering system of the polycyclic ring system component is retained with one system having primed locants. The location of the spiro atom is indicated in the name by the appropriate locants (unprimed first) placed at the front of the name.

Example:

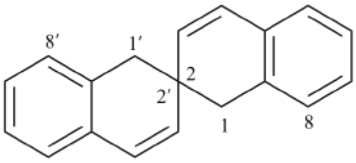


7,7′-spirobi[bicyclo[4.1.0]heptane] (PIN)

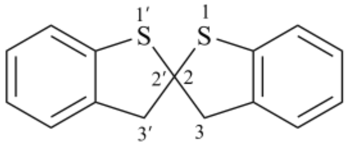
P-24.3.2 Where appropriate the maximum number of noncumulative double bonds is added (i.e., the system is made mancude) after construction of the complete skeleton. Indicated hydrogen (P-14.7) of individual components is not cited (ref. 8). No indicated hydrogen is cited when none is present in the spiro system. If indicated hydrogen is needed, it is cited in front of the spiro atom locants.

Note: This treatment of indicated hydrogen was introduced in the 1999 publication on the nomenclature of spiro compounds (ref. 8)

Examples:

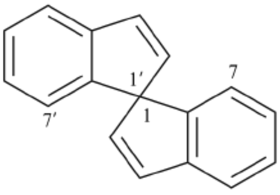


1*H*,1′*H*-2,2′-spirobi[naphthalene] (PIN)

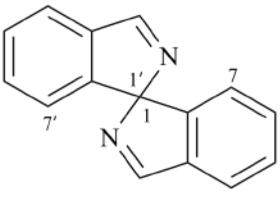


3*H*,3′*H*-2,2′-spirobi[[1]benzothiophene] (PIN)

Note: The double set of brackets in this name occurs because the spiro name requires them and brackets are used to enclose locants belonging to component names (see P-16.5.2.2).



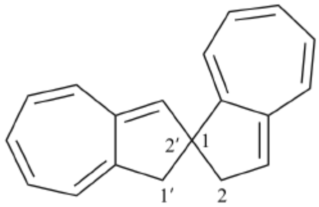
1,1′-spirobi[indene] (PIN)



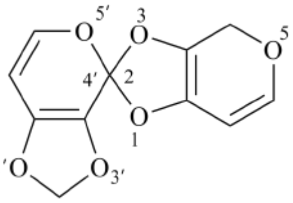
1,1′-spirobi[isoindole] (PIN)

P-24.3.3 If there is a choice for assigning primed locants, the lower number at the spiro atom is unprimed.

Examples:

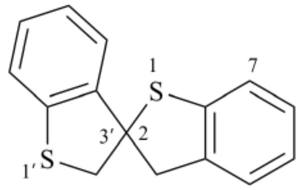


1′*H*,2*H*-1,2′-spirobi[azulene] (PIN)



2′*H*,4*H*-2,4′-spirobi[[1,3]dioxolo[4,5-*c*]pyran] (PIN)

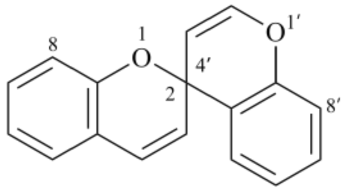
Note: The double set of brackets in this name occurs because the spiro name requires them and brackets are used to enclose locants belonging to component names (see P-16.5.2.2).



2′*H*,3*H*-2,3′-spirobi[[1]benzothiophene] (PIN)

Note 1: The indicated hydrogen at position 2′ may be omitted in general nomenclature, but it must be cited in the preferred IUPAC name.

Note 2: The double set of brackets in this name occurs because the spiro name requires them and brackets are used to enclose locants belonging to component names (see P-16.5.2.2).



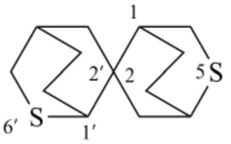
2,4′-spirobi[[1]benzopyran] (PIN)
2,4′-spirobi[chromene]

P-24.3.4 Heterocyclic ‘spirobi’ ring systems named by skeletal replacement (‘a’) nomenclature

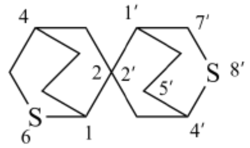
When ring components of ‘spirobi’ compounds are named by von Baeyer nomenclature, heteroatoms are indicated by skeletal replacement (‘a’) nomenclature. The spirobi ring system is named as the saturated bi- or polycyclic alicyclic hydrocarbon and the heteroatoms are denoted by ‘a’ prefixes cited at the front of the completed ‘spirobi’ hydrocarbon name. If there is a choice, low locants are given to the spiro atom, then to the heteroatoms as described in Section P-24.2.4.1.

Note: This treatment of skeletal replacement (‘a’) prefixes was introduced in the 1999 publication on the nomenclature of spiro compounds (ref. 8).

Examples:



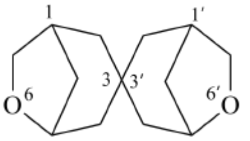
not



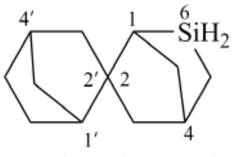
(**I**)
correct

(**II**)
incorrect

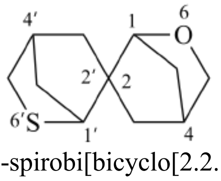
5,6′-dithia-2,2′-spirobi[bicyclo[2.2.2]octane] (**I**) (PIN)
[not 6,8′-dithia-2,2′-spirobi[bicyclo[2.2.2]octane] (**II**);
the set of locants ‘5,6′ ’ in (**I**) is lower than ‘6,8′ ’ in (**II**)]



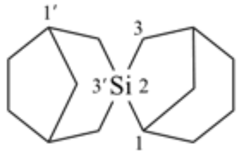
6,6′-dioxa-3,3′-spirobi[bicyclo[3.2.1]octane] (PIN)



6-sila-2,2′-spirobi[bicyclo[2.2.1]heptane] (PIN)



6-oxa-6′-thia-2,2′-spirobi[bicyclo[2.2.1]heptane] (PIN)

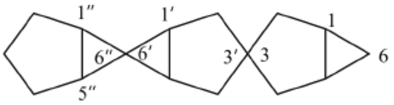


2-sila-2,3′-spirobi[bicyclo[3.2.1]octane] (PIN)

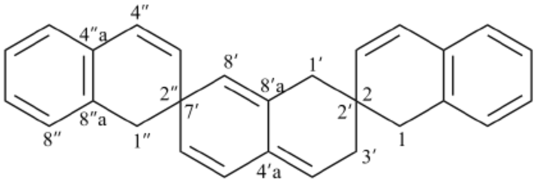
P-24.4 DISPIRO RING SYSTEMS WITH THREE IDENTICAL POLYCYCLIC RING SPIROFUSED TOGETHER

P-24.4.1 Dispiro ring systems with three identical polycyclic ring components are named by placing the nondetachable prefix ‘dispiroter’ before the name of the component ring system enclosed in square brackets. The multiplicative prefix ‘ter’ (see P-14.2.3) is used to indicate the repetition of identical ring components. Locants for the middle ring component are primed and for the third ring component double primed. The spiro atoms are indicated in front of the name by two pairs of locants separated by a colon. Indicated hydrogen is cited in front of these locants, if needed.

Examples:



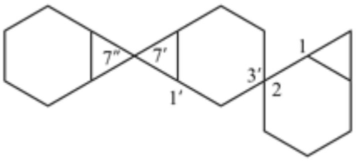
3,3′:6′,6″-dispiroter[bicyclo[3.1.0]hexane] (PIN)



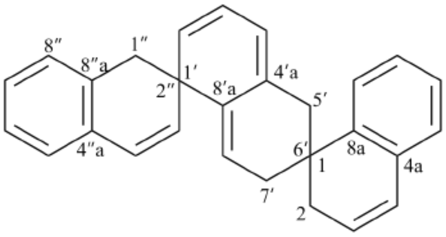
1*H*,1′*H*,1″*H*,3′*H*-2,2′:7′,2″-dispiroter[naphthalene] (PIN)

P-24.4.2 If there is a choice for locants, the lowest set of locants for all spiro atoms is selected when compared as a set in increasing order and, if there is a further choice, in their order of citation in the name.

Examples:

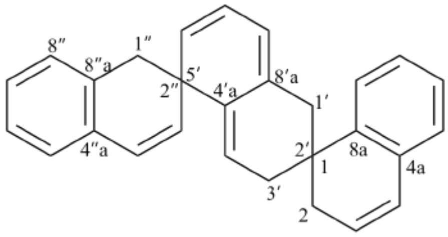


2,3′:7′,7″-dispiroter[bicyclo[4.1.0]heptane] (PIN)



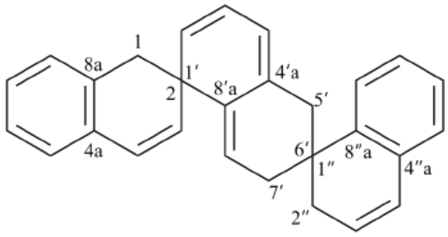
(I)
correct

not



(II)
incorrect

not



(III)

1″*H*,2*H*,5′*H*,7′*H*-1,6′:1′,2″-dispiroter[naphthalene] (**I**) (PIN)
[not 1′*H*,1″*H*,2*H*,3′*H*-1,2′:5′,2″-dispiroter[naphthalene] (**II**);
nor 1*H*,2″*H*,5′*H*,7′*H*-2,1′:6′,1″-dispiroter[naphthalene] (**III**)

Explanation: the locant set ‘1,1′,2″,6′ ’ in (**I**) is lower than ‘1,2′,2″,5′ ’ in (**II**) or ‘1′,1″,2,6′ ’ in (**III**).

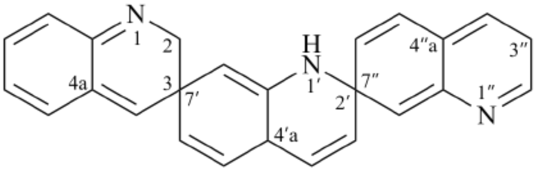
P-24.4.3 Three identical heterocyclic ring components spirofused together.

Dispiro compounds with three identical heterocyclic components may be named:

(a) by using heterocyclic monocyclic or polycyclic mancude components in the same way as for ‘spiroter’ hydrocarbons (see P-24.4.1); the numbering depends first on the fixed numbering of the heterocyclic components;

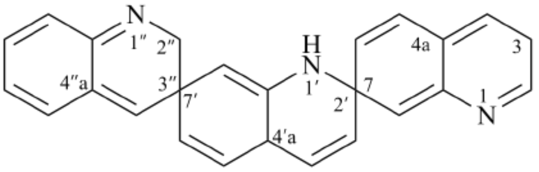
(b) by skeletal replacement (‘a’) nomenclature when the ring components are polycyclic von Baeyer ring systems; the numbering of the ‘spiroter’ von Baeyer hydrocarbon remains unchanged.

Examples:



correct

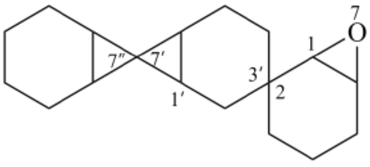
1′*H*,2*H*,3″*H*,4′a*H*-3,7′:2′,7″-dispiroter[quinoline] (PIN)



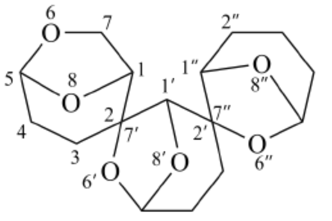
incorrect

1′*H*,2″*H*,3*H*,4′a*H*-7,2′:7′,3″-dispiroter[quinoline]

Explanation: The locant set ‘2′,3,7′,7″....’ in the correct name, the PIN, is lower than the locant set ‘2′,3″,7,7′... ’ in the incorrect name



7-oxa-2,3′:7′,7″-dispiroter[bicyclo[4.1.0]heptane] (PIN)



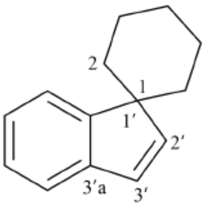
6,6′,6″,8,8′,8″-hexaoxa-2,7′:2′,7″-dispiroter[bicyclo[3.2.1]octane] (PIN)

P-24.5 MONOSPIRO RING SYSTEMS WITH DIFFERENT RING COMPONENTS, AT LEAST ONE OF WHICH IS A POLYCYCLIC RING SYSTEM

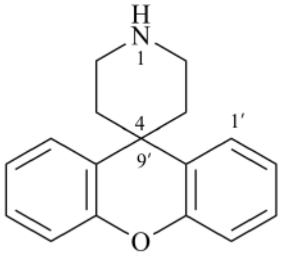
P-24.5.1 Monospiro ring systems with different ring components, at least one being a polycyclic ring system to which skeletal replacement (‘a’) nomenclature does not apply, are formed by placing the ring component names in alphanumerical order within square brackets. The position of the spiro atom is denoted by appropriate locants separated by a comma and placed between the names of the two ring components. Locants of the second ring component are primed and thus any locants needed to name it are placed in square brackets. Indicated hydrogen (see P-14.7) is cited in front of the name if needed in the complete structure (P-24.3.2).

Note: In naming polycyclic spiro ring systems consisting of different ring components, the first ring to be cited is determined by alphabetical order and not by seniority of the rings or ring systems.

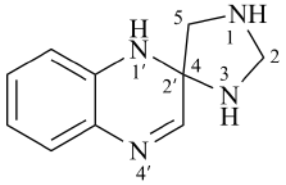
Examples:



spiro[cyclohexane-1,1′-indene] (PIN)
(no indicated hydrogen is required, see P-24.3.2)



spiro[piperidine-4,9′-xanthene] (PIN)
(no indicated hydrogen is required, see P-24.3.2)

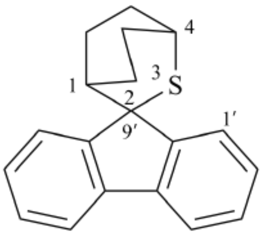


1′*H*-spiro[imidazolidine-4,2′-quinoxaline] (PIN)

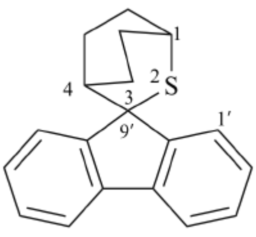
P-24.5.2 Monospiro ring systems with different ring components at least one being a polycyclic ring and at least one ring component requiring the use of skeletal replacement ('a') nomenclature are named as in P-24.5.1; then, the skeletal replacement ('a') prefixes are introduced and cited before the 'spiro' term.

Note: This treatment of skeletal replacement ('a') prefixes was introduced in the 1999 publication on the nomenclature of spiro compounds (ref. 8).

Examples:



not



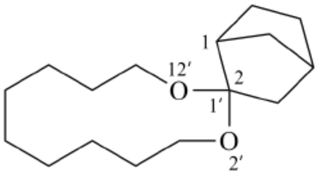
(**I**) correct

(**II**) incorrect

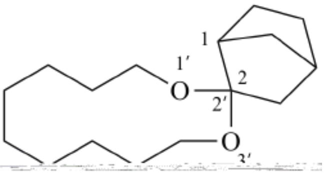
3-thiaspiro[bicyclo[2.2.2]octane-2,9′-fluorene] (**I**) (PIN)
[not 2-thiaspiro[bicyclo[2.2.2]octane-3,9′-fluorene] (**II**)]

Explanation: The locant set '2,9′ ' in (**I**) is lower than '3,9′ ' in (**II**).

Note: The format of the 'correct' name given in SP-4.1 in ref. 8, spiro[fluorene-9,2′-[3]thiabicyclo[2.2.2]octane], is no longer recommended.



not



(**I**) correct

(**II**) incorrect

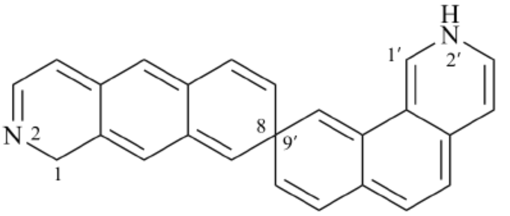
2′,12′-dioxaspiro[bicyclo[2.2.1]heptane-2,1′-cyclododecane] (**I**) (PIN)
[not 1′,3′-dioxaspiro[bicyclo[2.2.1]heptane-2,2′-cyclododecane] (**II**)]

Explanation: The spiro atom of the monocyclic hydrocarbon component is given preference for low locant.

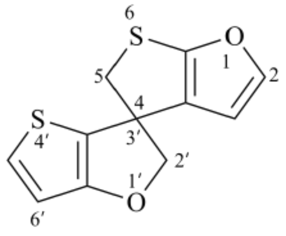
Note: The format of the 'correct' name given in SP-4.1, ref. 8,
spiro[bicyclo[2.2.1]heptane-2,1′-[2,12]dioxacyclododecane], is no longer recommended.

P-24.5.3 Alphanumerical order, as described in Section P-14.5 and P-14.6, is used when necessary. When Roman letters are inadequate to distinguish alphabetically between two ring components, criteria based on italic fusion letters and numbers, heteroatom locants, and von Baeyer descriptor numbers are used, as appropriate. All locants present in bicyclic fused benzo ring component or Hantzsch-Widman named component are placed in brackets (without primes for the second component, see third and fourth examples below).

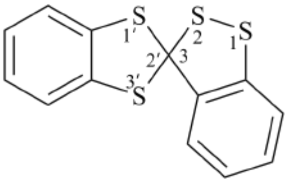
Examples:



1*H*,2′*H*-spiro[benzo[*g*]isoquinoline-8,9′-benzo[*h*]isoquinoline] (PIN)
(benzo[*g*].... before benzo[*h*]....)

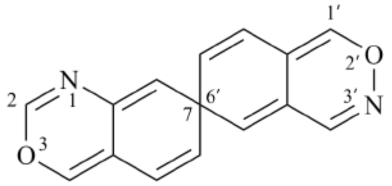


2′*H*,5*H*-spiro[thieno[2,3-*b*]furan-4,3′-thieno[3,2-*b*]furan] (PIN)
(...[2,3-*b*]... before ...[3,2-*b*]...)



spiro[[1,2]benzodithiole-3,2′-[1,3]benzodithiole] (PIN)
(1,2-benzo... before 1,3-benzo...)

Note: The double set of brackets in this name occurs because the spiro name requires them and brackets are used to enclose locants belonging to ring component names (see P-16.5.2.2). The use of brackets in the name of the first cited component is a change from SP-4 of ref. 8.

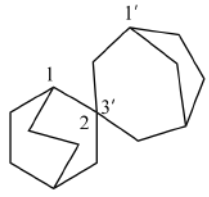


spiro[[3,1]benzoxazine-7,6′-[2,3]benzoxazine] (PIN)
(3,1-benzoxazine before 2,3-benzoxazine)

Note: The double set of brackets in this name occurs because the spiro name requires them and brackets are used to enclose locants belonging to ring component names (see P-16.5.2.2). The use of brackets in the name of the first cited component is a change from SP-4 of ref. 8.

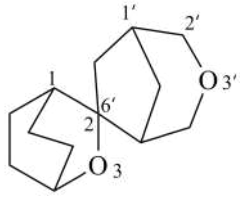
P-24.5.4 In the case of ring systems modified by skeletal replacement (‘a’) nomenclature, P-24.5.1 and P-24.5.3 are applied to name the ring system before skeletal replacement (‘a’) nomenclature is applied as described in P-24.5.2. The names of ring components modified by skeletal replacement (‘a’) nomenclature must not be used; thus P-24.5.3 must be applied when required.

Examples:

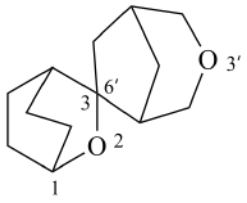


spiro[bicyclo[2.2.2]octane-2,3′-bicyclo[3.2.1]octane] (PIN)
[bicyclo[2.2.2]octane is cited before bicyclo[3.2.1]octane]

Explanation: The descriptor set ‘2.2.2’ is lower than ‘3.2.1’ (see P-14.3.5).



not



(**I**)
correct

(**II**)
incorrect

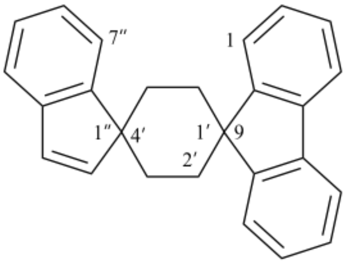
3,3′-dioxaspiro[bicyclo[2.2.2]octane-2,6′-bicyclo[3.2.1]octane] (**I**) (PIN)
[not 2,3′-dioxaspiro[bicyclo[2.2.2]octane-3,6′-bicyclo[3.2.1]octane] (**II**)]

Explanation: spiro fusion is preferred to replacement ('a') prefixes for low locants and the locant set 2,6′ in the PIN (**I**) is lower than 3,6′ in (**II**).

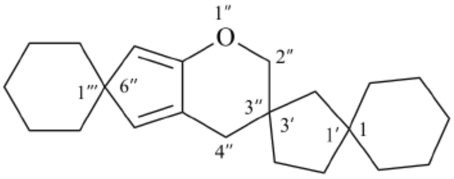
P-24.6 UNBRANCHED POLYSPIRO RING SYSTEMS WITH DIFFERENT RING COMPONENTS ONE BEING A POLYCYCLIC RING SYSTEM

Unbranched polyspiro ring systems with at least two different ring components and at least one of which is a polycyclic ring are named by placing the ring component names in order of their occurrence in the structure beginning with the terminal ring component lower in alphabetical order and enclosing within square brackets. A nondetachable prefix indicating the number of spiro atoms ('dispiro', 'trispiro', etc.) is placed in front of the enclosed ring component names. Locants of the first cited ring component are unprimed, the next ring component is primed, and so on. In a complete name, all locants present in a bicyclic fused benzo ring component or Hantzsch-Widman named component are placed in brackets (without primes for the second and subsequent components, see fourth example below). The positions of the spiro atoms are indicated by the appropriate pair of locants separated by a comma and placed between each pair of component ring system names. Indicated hydrogen is used as needed and cited in front of the 'dispiro', 'trispiro', etc., prefix. If both terminal ring systems are the same, the order for citation of ring system components is determined by comparing the pair of second ring components from the end of the structure, and so on (See section SP-5 in ref. 8 for further discussion).

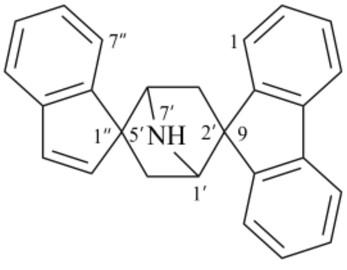
Examples:



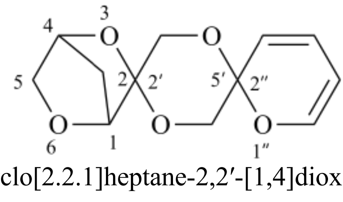
dispiro[fluorene-9,1′-cyclohexane-4′,1″-indene] (PIN)



2″*H*,4″*H*-trispiro[cyclohexane-1,1′-cyclopentane-3′,3″-cyclopenta[*b*]pyran-6″,1‴-cyclohexane] (PIN)



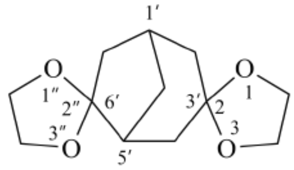
7′-azadispiro[fluorene-9,2′-bicyclo[2.2.1]heptane-5′,1″-indene] (PIN)



3,6-dioxadispiro[bicyclo[2.2.1]heptane-2,2′-[1,4]dioxane-5′,2″-pyran] (PIN)

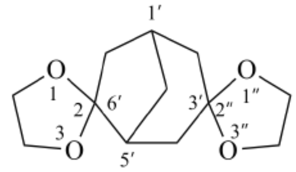
P-24.6.1 If there is a choice of locants, the lowest set of locants for all spiro atoms is selected when compared in increasing numerical order and, if there is still a choice, in order of their citation in the name (see P-24.2.4.1).

Example:



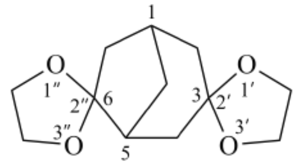
(I)
correct

not



(II)
incorrect

nor



(**III**)
incorrect

dispiro[[1,3]dioxolane-2,3′-bicyclo[3.2.1]octane-6′,2″-[1,3]dioxolane] (**I**) (PIN)
[not dispiro[[1,3]dioxolane-2,6′-bicyclo[3.2.1]octane-3′,2″-[1,3]dioxolane] (**II**);
the locant sets 2,2″,3′,6′ are identical, but in the name
the order of citation 2,3′,6′,2″ in the PIN (**I**) is lower than 2,6′,3′,2″ in (**II**)]
[not dispiro[bicyclo[3.2.1]octane-3,2′:6,2″-bis([1,3]dioxolane) (**III**) (see P-24.4.2)]

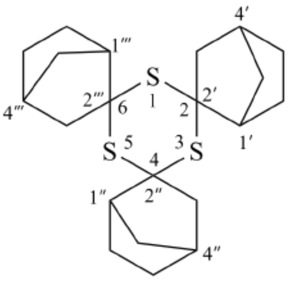
Note 1: The double set of brackets in the traditional name above occurs because the spiro name requires them and brackets are used to enclose locants belonging to ring component names (see P-16.5.2.2). The use of brackets in the name of the first cited component is a change from SP-4 of ref. 8.

P-24.7 BRANCHED POLYSPIRO RING SYSTEMS

When three or more components are spirofused to another single component, the system is described as a branched spirofused system. Terminal components have only one spiro atom.

P-24.7.1 When a central ring component is spirofused to three or more identical terminal ring components, the central ring component is cited first and its locants are unprimed. The terminal ring components are cited with the appropriate multiplicative prefix (‘tris’, ‘tetrakis’, etc.) and their locants are primed, double primed, etc., in accordance with the lowest possible locants of the spiro atoms of the central ring component. The spiro atoms are indicated by pairs of locants separated by a colon. Indicated hydrogen is cited as necessary in front of the appropriate spiro prefix.

Example:

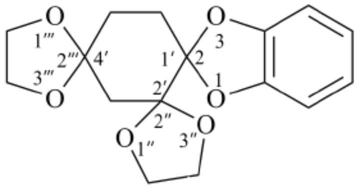


trispiro[[1,3,5]trithiane-2,2′:4,2″:6,2‴-tris(bicyclo[2.2.1]heptane)] (PIN)

P-24.7.2 When two or more different terminal ring components are spirofused to a central component, the alphabetically earliest is cited first with a multiplicative prefix, if appropriate, followed by the central ring component and then the remaining terminal ring component(s) in alphabetical order. The first cited ring component, or one of the first cited ring components, is spirofused to the lowest numbered spiro position of the central ring component; then lowest locants are assigned to the remaining terminal ring components according to their alphabetical order (including other first cited ring components if more than one).

Examples:

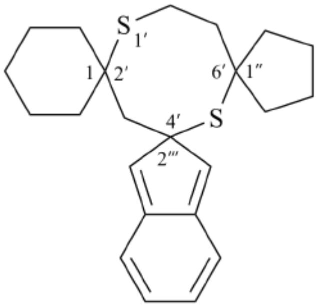
(1)



trispiro[[1,3]benzodioxole-2,1′-cyclohexane-2′,2″:4′,2‴-bis([1,3]dioxolane)] (PIN)

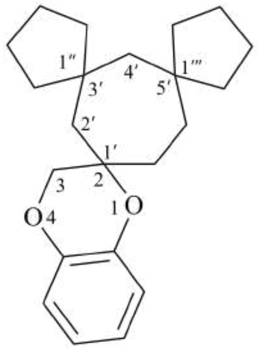
Note: The double set of brackets in this name occurs because the spiro name requires them and brackets are used to enclose locants belonging to ring component names (see P-16.5.2.2). The use of brackets in the name of the first cited component is a change from SP-4 of ref. 8.

(2)



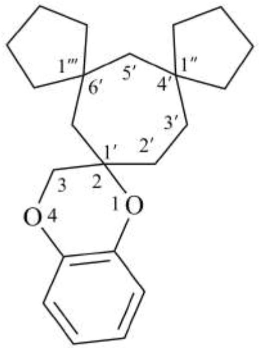
trispiro[cyclohexane-1,2′-[1,5]dithiocane-6′,1″-cyclopentane-4′,2‴-indene] (PIN)
(the cyclohexane ring must be spirofused at position ‘2’ of the dithiocane central ring component)

(3)



(I)
correct

not

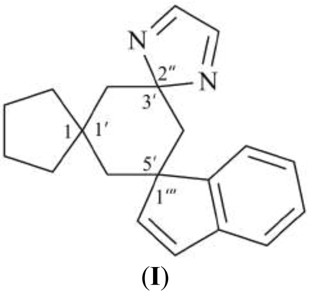


(II)
incorrect

3*H*-trispiro[[1,4]benzodioxine-2,1′-cycloheptane-3′,1″:5′,1‴-bis(cyclopentane)] (**I**) (PIN)
{not 3*H*-trispiro[[1,4]benzodioxine-2,1′-cycloheptane-4′,1″:6′,1‴-bis(cyclopentane)] (**II**)}

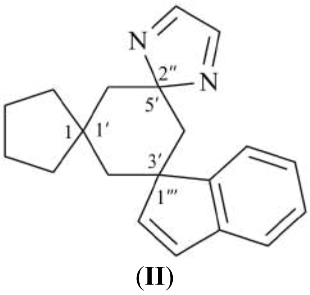
Explanation: the first cited component is the alphabetically earliest, 1,4-benzodioxine, which determines the locant 1′ of the central ring component cycloheptane. The set of spirofusion locants 1′,3′,5′ in (**I**) is lower than 1′,4′,6′ in (**II**).

(4)



(I)
correct

not



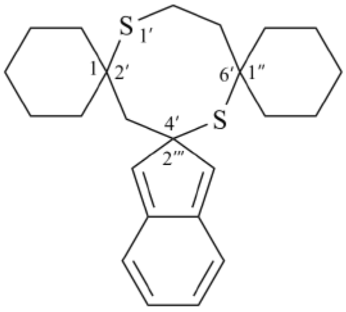
(II)
incorrect

trispiro[cyclopentane-1,1′-cyclohexane-3′,2″-imidazole-5′,1‴-indene] (**I**) (PIN)
[not trispiro[cyclopentane-1,1′-cyclohexane-5′,2″-imidazole-3′,1‴-indene] (**II**)

Explanation: The locant 3′ in (**I**) is lower than 5′ in (**II**) for the first cited ring component following the citation of the central ring component.

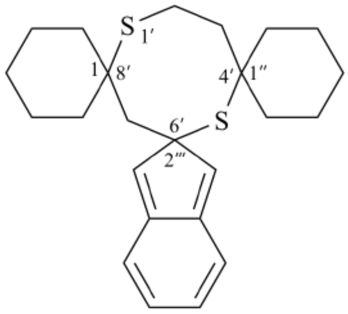
P-24.7.3 If no decision can be attained by application of P-24.7.2 and if there is a choice of locants, the lowest set of locants for all spiro atoms is selected when compared as a set in increasing numerical order, and, if still undecided, in their order of their citation in the name. If a choice still remains, criteria about heteroatoms and indicated hydrogen are taken into consideration (see Section SP-3.2 in ref. 8).

Example:



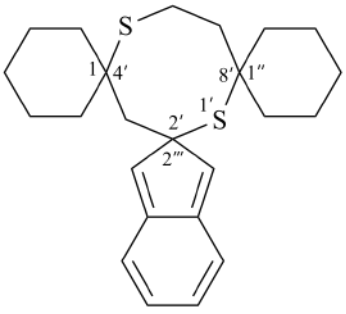
(I)
correct

not



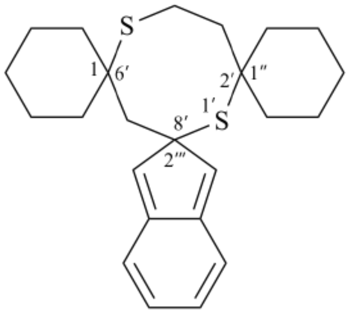
(II)
incorrect

nor



(III)
incorrect

nor



(IV)
incorrect

trispiro[bis(cyclohexane)-1,2′:6′,1″-[1,5]dithiocane-4′,2‴-indene] (**I**) (PIN)
[not trispiro[bis(cyclohexane)-1,8′:4′,1″-[1,5]dithiocane-6′,2‴-indene] (**II**)
nor trispiro[bis(cyclohexane)-1,4′:8′,1″-[1,5]dithiocane-2′,2‴-indene] (**III**);
nor trispiro[bis(cyclohexane)-1,6′:2′,1″-[1,5]dithiocane-8′,2‴-indene] (**IV**)]

Explanation: The locant set 1,1″,2′,2‴,4′,6′ in (**I**) is lower than 1,1″,2‴,4′,6′,8′ in (**II**), 1,1″,2′,2‴,4′,8′ in (**III**), or 1,1″,2′,2‴,6′,8′ in (**IV**).

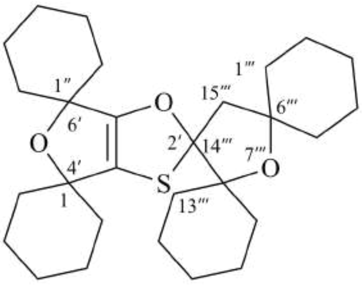
P-24.7.4 If additional components are spiro-fused to a branched polyspiro compound as described in P-24.7.1 to P-24.7.3, the following criteria are applied in order:

(a) Any monocyclic ring components spirofused together including skeletal replacement (‘a’) prefixes, if any, are named (P-24.2) as a unit containing the maximum number of monocyclic ring components. The unit is used as a component for further spiro-fusion (see P-24.6). To help indicate the composite nature of the name braces are used (instead of brackets) after the initial polyspiro prefix to enclose components at least one of which is already spiro-fused;

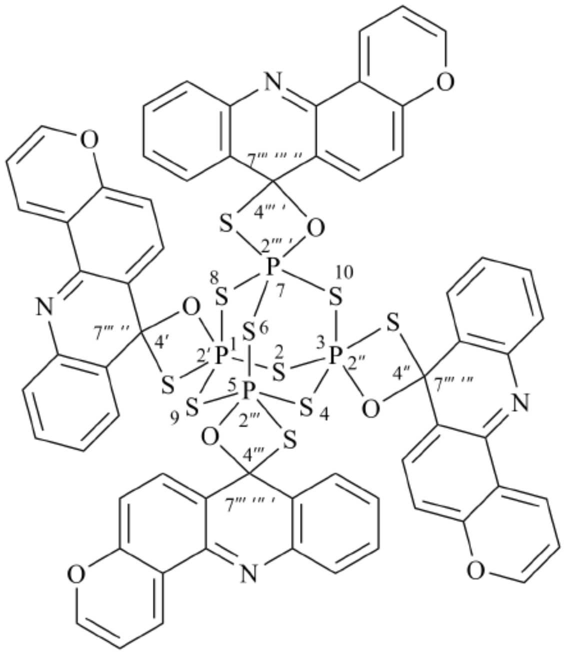
(b) If there is not a polyspiro system of monocyclic ring components or the system cannot be named by the normal spiro-fusion described previously the largest spiro system is named and treated as a unit for further spiro-fusion. The priming of the unit is continued to the rest of the name.

P-24.7.4.1 After identification of the spiro-fused components these, together with the remaining components, are treated in the normal way.

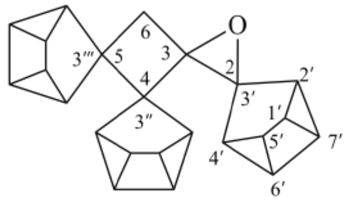
Examples:



trispiro{bis(cyclohexane)-1,4′:1″,6′-furo[3,4-*d*][1,3]oxathiole-2′,14‴-[7]oxadispiro[$5.1.5^8.2^6$]pentadecane} (PIN)
pentaspiro[tetracyclohexane-1,2′(5′*H*):1‴,5′:1⁗,4″(6″*H*):1′′′′′,6″-furan-3′(4′*H*),2″-furo[3,4-*d*][1,3]oxathiole]
(the CAS index name; note that multiple primes are not divided into groups of three)



1λ^{5},3λ^{5},5λ^{5},7λ^{5}-tetraspiro{tetraspiro[2,4,6,8,9,10-hexathia-1,3,5,7-tetraphosphaadamantane-1,2′:3,2″:5,2‴:7,2‴′-tetrakis([1,3,2]oxathiaphosphetane)-4′,7‴″:4″,7‴‴:4‴,7‴‴′:4‴′,7‴‴″-tetrakis(pyrano[2,3-*c*]acridine)}
[PIN, see SP-6.4 (b) in ref 8]
octaspiro[2,4,6,8,9,10-hexathia-1,3,5,7-tetraphosphatricyclo[3.3.1.1^{3,7}]decane-1,2′λ^{5}:3,2″λ^{5}:5,2‴λ^{5}:7,2′′′′λ^{5}-tetrakis[1,3,2]oxathiaphosphetane-4′,7′′′′′:4″,7′′′′′′:4‴,7′′′′′′′:4′′′′,7′′′′′′′′-tetrakis[7*H*]pyrano[2,3-*c*]acridine]
(the CAS index name; note that multiple primes are not divided into groups of three)



trispiro{1-oxaspiro[2.3]hexane-2,3′:4,3″:5,3‴-tris(tetracyclo[3.2.0.0^{2,7}.0^{4,6}]heptane)} (PIN)

P-24.8 SPIRO RING SYSTEMS CONTAINING ATOMS WITH NONSTANDARD BONDING NUMBERS

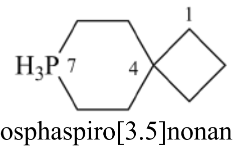
The λ-convention, characterized by the symbol λ^{n}, is used to identify heteroatoms with nonstandard bonding numbers (see P-14.1). The symbol is placed at the front of the complete name or before the skeletal replacement (‘a’) prefix for the atom to which it refers.

P-24.8.1 Spiro ring systems with only monocyclic ring components
P-24.8.2 Monospiro ring systems with two identical polycyclic ring components
P-24.8.3 Spiro ring systems with three identical components and one nonstandard spiro atom
P-24.8.4 Monospiro ring systems with different ring components, at least one of which is a polycyclic ring with a nonstandard spiro atom
P-24.8.5 Unbranched polyspiro ring systems with different ring components, at least one of which is a polycyclic ring with at least one nonstandard spiro atom
P-24.8.6 Branched spiro ring systems with at least one polycyclic ring component

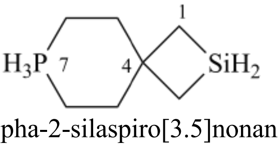
P-24.8.1 Spiro ring systems with only monocyclic ring components

P-24.8.1.1 Heteroatoms having nonstandard bonding numbers receive lowest locants in accordance with the numbering of the corresponding spiro ring system.

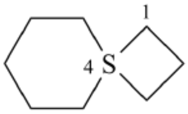
Examples:



7λ^{5}-phosphaspiro[3.5]nonane (PIN)



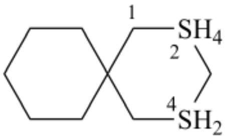
7λ^{5}-phospha-2-silaspiro[3.5]nonane (PIN)



$4\lambda^4$-thiaspiro[3.5]nonane (PIN)

P-24.8.1.2 If there is a choice, lower locants are assigned to heteroatoms with the higher bonding number, for example, the lower number is assigned to a λ^6 heteroatom rather than to a λ^4 heteroatom.

Example:

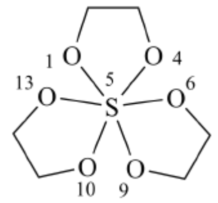


$2\lambda^6,4\lambda^4$-dithiaspiro[5.5]undecane (PIN)

P-24.8.1.3 Spiro ring systems composed of only three monocyclic rings and a nonstandard spiro atom are named by extending the rules for naming spiro ring systems as defined in P-24.1.

P-24.8.1.3.1 Ring systems consisting of three monocyclic rings and one nonstandard spiro atom (e.g., a λ^6 spiro atom) are named by placing the prefix ‘spiro’ before the name corresponding to an alicyclic system with the same total number of skeletal atoms in the spiro ring system. Heteroatoms are indicated by ‘a’ prefixes and the nonstandard bonding number by the ‘λ’ symbol (see P-14.1). In the von Baeyer spiro descriptor, the locant of the spiro atom is used as a superscript number to indicate each time the spiro atom is revisited.

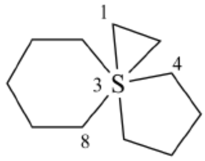
Example:



1,4,6,9,10,13-hexaoxa-$5\lambda^6$-thiaspiro[$4.4^5.4^5$]tridecane (PIN)

P-24.8.1.3.2 If there is a choice for numbering, a small ring is numbered before a larger ring.

Example:

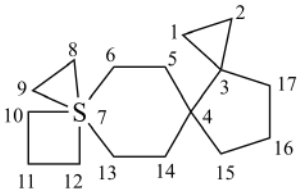


$3\lambda^6$-thiaspiro[$2.4^3.5^3$]dodecane (PIN)

P-24.8.1.4 Polyspiro ring systems which include at least three monoalicyclic rings with one nonstandard hetero spiro atom as well as other spiro fusions are named by extending the rules for naming spiro ring systems as defined in P-24.1. They are named using a combination of methods for naming the polyspiro ring systems and for indicating heteroatoms with nonstandard bonding numbers. If there is a choice for numbering, the following criteria are considered in order until a decision is made:

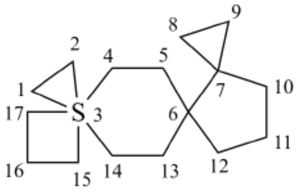
(a) Low numbers are selected for spiro atoms;

Example:



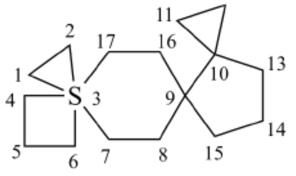
(I)
correct

not



(II)
incorrect

nor



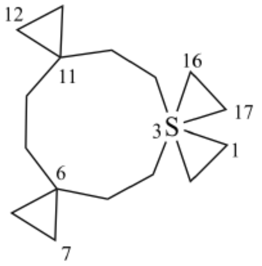
(III)
incorrect

$7\lambda^6$-thiatrispiro[$2.0.2.2^7.3^7.2^4.3^3$]heptadecane (**I**) (PIN)
[not $3\lambda^6$-thiatrispiro[$2.2.0.2^7.3^6.2^3.3^3$]heptadecane (**II**);
nor $3\lambda^6$-thiatrispiro[$2.3.2.0.2^{10}.3^9.2^3$]heptadecane (**III**)]

Explanation: The locant set for the spiro atoms in (**I**), ‘3,4,7’, is lower than ‘3,6,7’ in (**II**) or ‘3,9,10’ in (**III**).

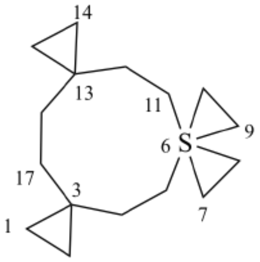
(b) Low numbers are selected for spiro atoms connecting three rings;

Example:



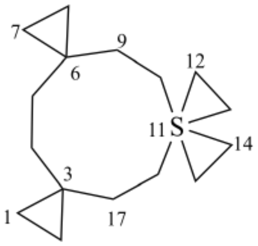
(**I**)
correct

not



(**II**)
incorrect

nor



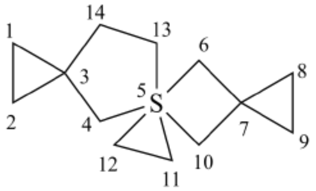
(**III**)
incorrect

$3\lambda^6$-thiatrispiro[$2.2.2^6.2.2^{11}.2^3.2^3$]heptadecane (**I**) (PIN)
[not $6\lambda^6$-thiatrispiro[$2.2.2^6.2^6.2.2^{13}.2^3$]heptadecane (**II**);
nor $11\lambda^6$-thiatrispiro[$2.2.2^6.2.2^{11}.2^{11}.2^3$]heptadecane (**III**)]

Explanation: The locant '3' for the spiro atom connecting three rings in (**I**) is lower than '6' in (**II**) or '11' in (**III**).

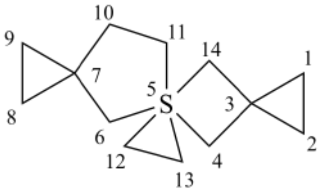
(c) Low numbers are selected for the von Baeyer spiro descriptor in order of citation;

Example:



(**I**)
correct

not



(**II**)
incorrect

$5\lambda^6$-thiatrispiro[$2.1.1.2^7.1^5.2^5.2^3$]tetradecane (**I**) (PIN)
[not $5\lambda^6$-thiatrispiro[$2.1.1.2^7.2^5.2^5.1^3$]tetradecane (**II**)]

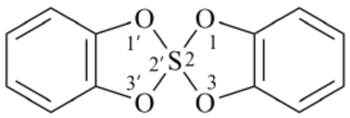
Explanation: The spirodescriptor set '2,1,1,2,1,2,2' in (**I**) is lower than '2,1,1,2,2,2,1' in (**II**).

P-24.8.2 Monospiro ring systems with two identical polycyclic ring components

The λ^n symbol is placed at the front of the complete name formed from the names of two identical ring system components including the heteroatoms in their name; the λ^n symbol is preceded by the lowest locant denoting the spiro atom. If indicated hydrogen atoms are required, they are placed before the λ symbol. When there is a choice, the locant of the first cited component is used for indicated hydrogen.

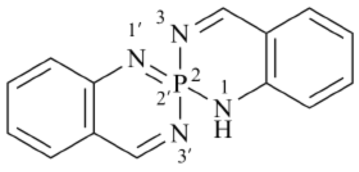
Note: The 'lowest locant' is used as the criterion for identification of the λ^n spiro atom rather than 'least primed locant' as used in SP-7 in ref. 8.

Examples:



$2\lambda^4,2'$-spirobi[[1,3,2]benzodioxathiole] (PIN)

Note: The double set of brackets in this name occurs because the spiro name requires them (see P-24.3.1) and brackets are used to enclose locants belonging to ring component names (see P-16.5.2.2).



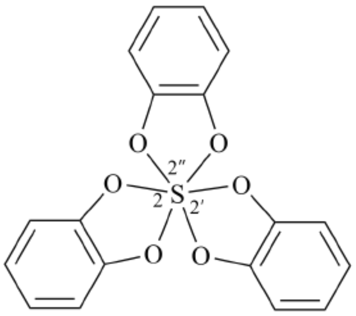
1*H*-$2\lambda^5,2'$-spirobi[[1,3,2]benzodiazaphosphinine] (PIN)

Note: The double set of brackets in this name occurs because the spiro name requires them (see P-24.3.1) and brackets are used to enclose locants locants belonging to ring component names (see P-16.5.2.2).

P-24.8.3 Spiro ring systems with three identical components and one nonstandard spiro atom.

Ring systems composed of three identical polycyclic ring components and only one spiro atom are named by placing the prefix ‘spiroter’ before the name of the polycyclic component enclosed in square brackets. The three spiro locants are cited at the front of the name preceded by the λ symbol with its locant that must be the lowest of the three denoting the spiro atom.

Example:



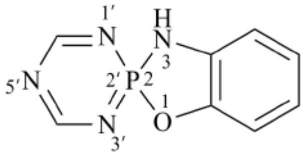
2λ^{6},2′,2″-spiroter[[1,3,2]benzodioxathiole] (PIN)

Note: The double set of brackets in this name occurs because the spiro name requires them and brackets are used to enclose locants belonging to ring component names (see P-16.5.2.2).

P-24.8.4 Monospiro ring systems with different ring components at least one of which is a polycyclic ring with a nonstandard spiro atom

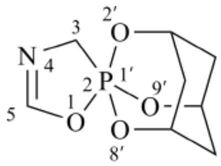
P-24.8.4.1 Monospiro ring systems composed of two different ring systems and a spiro heteroatom with a nonstandard bonding number are named by placing the prefix spiro in front of the names of the components cited in alphabetical order and with appropriate spiro locants. The lowest locant (unprimed) is used to denote the spiro fusion and the λ symbol is placed at the front of the name. Indicated hydrogen, if necessary, is added in front of the λ symbol. Any additional atom with a nonstandard bonding number is treated as a part of the name of the heterocycle; the λ symbol is cited with the lowest locant denoting the spiro atom.

Examples:



3*H*-2λ^{5}-spiro[[1,3,2]benzoxazaphosphole-2,2′-[1,3,5,2]triazaphosphinine] (PIN)

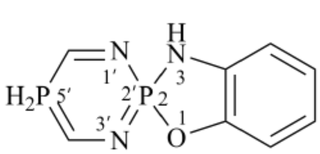
Note: The double set of brackets in this name occurs because the spiro name requires them and brackets are used to enclose locants belonging to ring component names (see P-16.5.2.2). The use of brackets in the name of the first cited component is a change from SP-4 of ref. 8.



3*H*-1′λ^{5}-spiro[[1,4,2]oxazaphosphole-2,1′-[2,8,9]trioxa[1]phosphaadamantane] (PIN)
3*H*-1′λ^{5}-spiro[[1,4,2]oxazaphosphole-2,1′-[2,8,9]trioxa[1]phosphatricyclo[3.3.1.1^{3,7}]decane]

Note 1: Adamantane, a retained name, is preferred to its systematic von Baeyer name.

Note 2: The double set of brackets in this name occurs because the spiro name requires them and brackets are used to enclose locants belonging to ring component names (see P-16.5.2.2). The use of brackets in the name of the first cited component is a change from SP-4 of ref. 8.

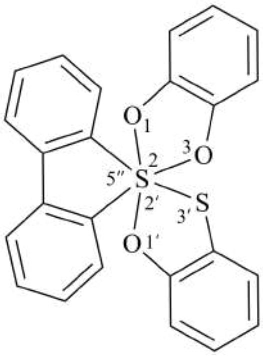


3*H*-2λ^{5},5′λ^{5}-spiro[[1,3,2]benzoxazaphosphole-2,2′-[1,3,2,5]diazadiphosphinine] (PIN)

Note: The double set of brackets in this name occurs because the spiro name requires them and brackets are used to enclose locants belonging to ring component names (see P-16.5.2.2). The use of brackets in the name of the first cited component is a change from SP-4 of ref. 8.

P-24.8.4.2 When three ring components represented by two different individual rings, are present, the name of the ring component that is cited second is placed in parentheses to highlight this unusual situation. The λ*ⁿ* symbol is placed at the front of the name, preceded by the lowest locant denoting the spiro atom.

Example:

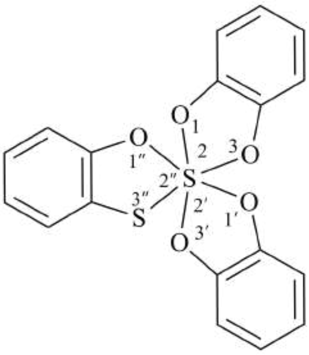


2λ⁶-spiro[[1,3,2]benzodioxathiole-2,2′-([1,2,3]benzoxadithiole)-2,5″-dibenzo[*b*,*d*]thiophene] (PIN)

Note: The double set of brackets in this name occurs because the spiro name requires them and brackets are used to enclose locants belonging to ring component names (see P-16.5.2.2). The use of brackets in the name of the first cited component is a change from SP-4 of ref. 8.

P-24.8.4.3 Two identical ring components are denoted by the prefix 'bis'. The λ*ⁿ* symbol is placed at the front of the name, preceded by the lowest locant denoting the spiro atom.

Example:



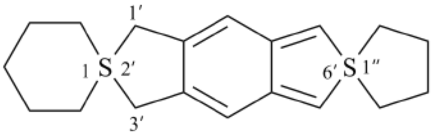
2λ⁶-spiro[bis([1,3,2]benzodioxathiole)-2,2″:2′,2″-[1,2,3]benzoxadithiole] (PIN)

Note: The double set of brackets in this name occurs because the spiro name requires them and brackets are used to enclose locants belonging to ring component names (see P-16.5.2.2).

P-24.8.5 Unbranched polyspiro ring systems with different ring components at least one of which is a polycyclic ring with at least one nonstandard spiro atom

Unbranched polyspiro ring systems with different ring components at least one of which is a polycyclic ring system with at least one nonstandard spiro atom are named using the method described in P-24.6. The λ-symbol denoting a spiro junction is associated with the lowest locant and placed in front of the name; it is preceded by indicated hydrogen(s), as needed.

Example:

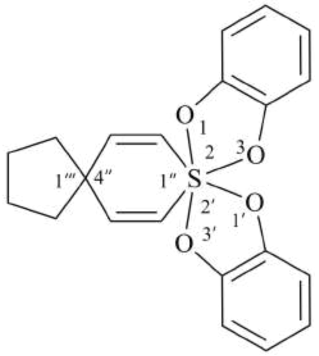


1′*H*,3′*H*-1λ⁴,1″λ⁴-dispiro[thiane-1,2′-benzo[1,2-*c*:4,5-*c*′]dithiophene-6′,1″-thiolane] (PIN)

P-24.8.6 Branched spiro ring systems with at least one polycyclic ring component

If two or more different terminal ring components are spirofused to a central ring component, the alphabetically earliest is cited first with multiplicative prefixes, if appropriate, followed by the central ring component and the remaining terminal ring components in alphabetical order. The λ symbol is placed at the front of the complete name and is denoted by the lowest spiro locant; it is preceded by indicated hydrogen, if needed.

Example:

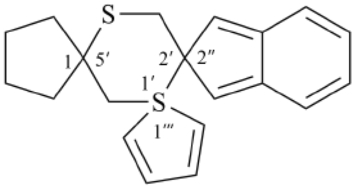


1″λ^6-dispiro[bis([1,3,2]benzodioxathiole)-2,1″:2′,1″-thiopyran-4″,1‴-cyclopentane] (PIN)

Note: The double set of brackets in this name occurs because the spiro name requires them and brackets are used to enclose locants belonging to ring component names (see P-16.5.2.2).

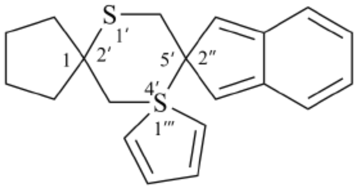
When there is a choice for locants, the lowest set of locants for all spiro atoms is selected, first by comparing them as a set in increasing numerical order, and, if still undecided, in the order of citation in the name. If a choice still remains, criteria involving the heteroatoms and indicated hydrogen atoms are taken into consideration (see Section SP-3.2 and SP-1.8 in ref. 8).

Example:



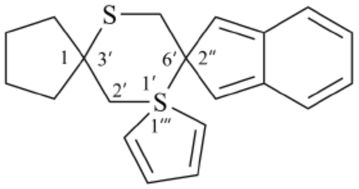
(**I**)
correct

not



(**II**)
incorrect

nor



(III)
incorrect

1′λ^4-trispiro[cyclopentane-1,5′-[1,4]dithiane-2′,2″-indene-1′,1″-thiophene] (**I**) (PIN)
[not 4′λ^4-trispiro[cyclopentane-1,2′-[1,4]dithiane-5′,2″-indene-4′,1‴-thiophene] (**II**)]
nor 1′λ^4-trispiro[cyclopentane-1,3′-[1,4]dithiane-6′,2″-indene-1′,1‴-thiophene] (**III**)]

Explanation: The locant set ‘1,1′,1‴,2′,2″,5′ ’ in (**I**) is lower than ‘1,1‴,2′,2″,4′,5′ ’ in (**II**), or ‘1,1′,1‴,2″,3′,6′ ’ in (**III**).

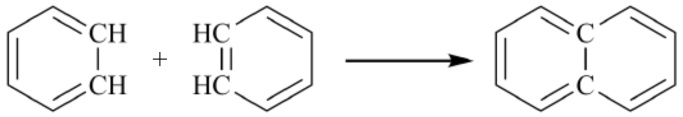
P-25 FUSED AND BRIDGED FUSED RING SYSTEMS

P-25.0 Introduction
P-25.1 Names of hydrocarbon parent ring components
P-25.2 Names of heterocyclic parent ring components
P-25.3 Constructing fusion names
P-25.4 Bridged fused ring systems
P-25.5 Limitations of fusion nomenclature: three components *ortho*- and *peri*-fused together
P-25.6 Fused ring systems with skeletal atoms with nonstandard bonding numbers
P-25.7 Double bonds, indicated hydrogen, and the δ-convention
P-25.8 Parent components in decreasing order of seniority (partial lists)

P-25.0 INTRODUCTION

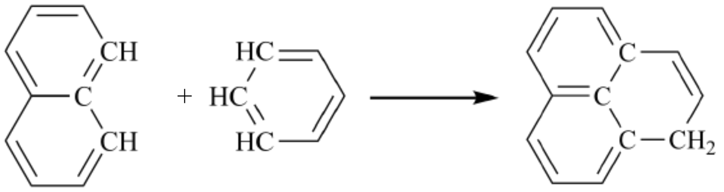
This section is based on the document entitled ‘Nomenclature of Fused and Bridged Fused Ring Systems, IUPAC Recommendations 1998’ (ref. 4).

In nomenclature, fusion is the operation that creates a common bond between two rings, each ring contributing one bond and the two atoms directly attached to the bond. This type of fusion is called *ortho*- or *ortho*- and *peri*-fusion if two adjacent bonds are involved. Atoms common to two or more rings are termed ‘fusion’ atoms. The term fusion is also used to describe the operation creating a common atom between two rings or ring systems, each contributing one atom. This type of fusion is called spirofusion (see P-24.1). Traditionally, *ortho*- and *ortho*- and *peri*-fusion were simply called fusion and the resulting polycyclic systems were referred to as fused ring systems or fused ring compounds. The term ‘spirofusion’ is new in nomenclature, and to avoid ambiguity ‘fusion’ should not be used without the prefix ‘spiro’ when ‘spirofusion’ is intended.



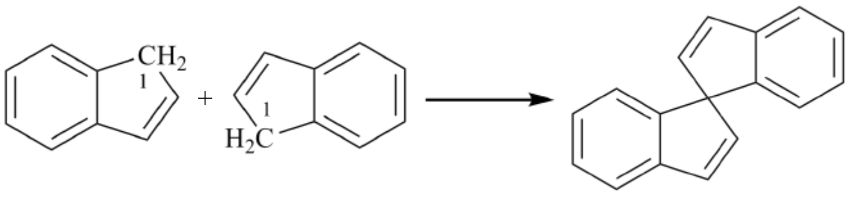
benzene (PIN) benzene (PIN) naphthalene (PIN)

Explanation: Naphthalene results from the fusion (*ortho*-fusion) of two benzene rings (one bond and two atoms in common).



naphthalene (PIN) benzene (PIN) 1*H*-phenalene (PIN)

Explanation: 1*H*-Phenalene results from the *ortho*- and *peri*-fusion of a naphthalene ring system and a benzene ring (two bonds and three atoms in common).



1*H*-indene (PIN) 1*H*-indene (PIN) 1,1′-spirobi[indene] (PIN)

Explanation: Spirobi[indene] results from the spirofusion of two indene ring systems (one atom in common)

This section deals with fused (*ortho*- and *ortho*- and *peri*-fused) ring systems and bridged fused (*ortho*- and *ortho*- and *peri*-fused) ring systems. Spirofusion is described in Section P-24. This section is intended only as an introduction to the vast field of fusion nomenclature discussed in the document entitled ‘Nomenclature of Fused and Bridged Fused Ring Systems’ (ref. 4). The principles presented herein use rather simple examples; for more complex ring systems the publication noted above or the ‘Ring Systems Handbook’, published by the Chemical Abstracts Service (ref. 22), should be consulted. Changes from previous rules are highlighted.

P-25.1 NAMES OF HYDROCARBON PARENT RING COMPONENTS

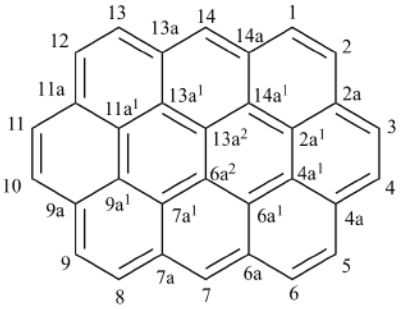
P-25.1.1 Retained names for hydrocarbons used for parent ring components and as attached ring components
P-25.1.2 Systematically named hydrocarbon parent components

P-25.1.1 Retained names for hydrocarbons used for parent ring components and as attached ring components

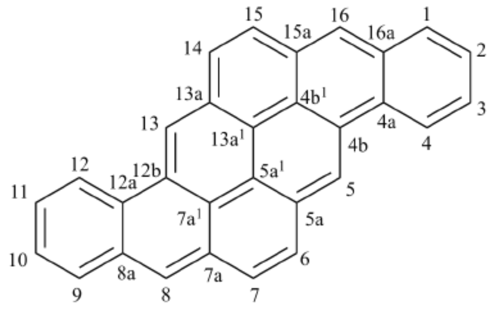
Retained names (also called trivial names) for polycyclic hydrocarbons are listed in Table 2.7, in decreasing order of seniority for being chosen as parent components in fusion nomenclature. Their numbering is indicated as the result of the application of the specific criteria used to number fused ring systems described in Section P-25.3.3.

Table 2.7 Retained names for hydrocarbon parent ring components
in descending order of seniority

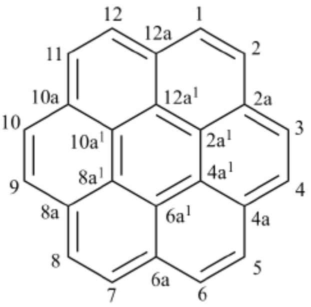
(the senority order is indicated by the number preceding the name;
the lower the number the higher the senority)



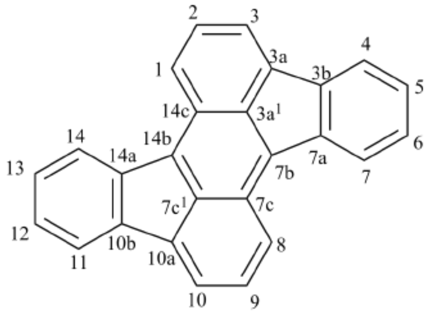
(1) ovalene (PIN)


15
15a
16
16a
1
14
2
13a
4b^{1}
3
13
13a^{1}
4a
4
4b
12
12b
5a^{1}
5
12a
11
7a^{1}
5a
10
6
8a
7a
9
8
7

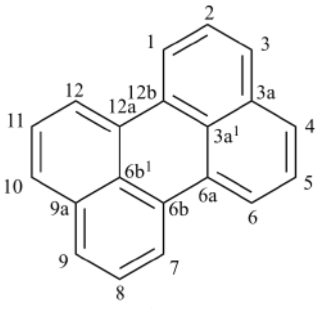
(2) pyranthrene (PIN)


12
1
12a
11
2
10a
12a^{1}
2a
10
3
10a^{1}
2a^{1}
9
8a^{1}
4a^{1}
4
8a
6a^{1}
4a
8
5
7
6a
6

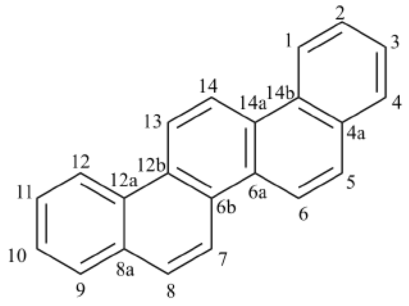
(3) coronene (PIN)


2
3
4
3a
3b
1
5
14c
3a^{1}
14
14b
6
7a
13
14a
7b
7
7c^{1}
7c
12
10b
8
11
10a
10
9

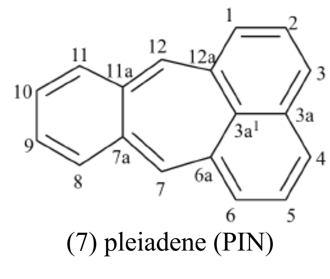
(4) rubicene (PIN)


2
1
3
12
3a
12b
12a
11
4
3a^{1}
6b^{1}
10
5
6a
9a
6b
6
9
7
8

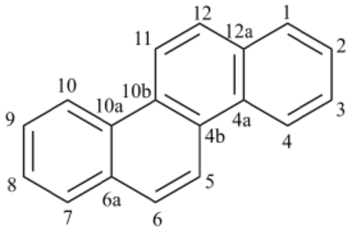
(5) perylene (PIN)


2
1
3
14
14a
14b
4
13
4a
12
12b
12a
5
11
6b
6a
6
10
7
9
8a
8

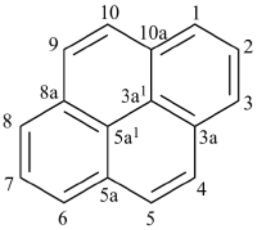
(6) picene (PIN)


1
2
11
12
12a
11a
3
10
3a
3a^{1}
9
7a
4
8
7
6a
6
5

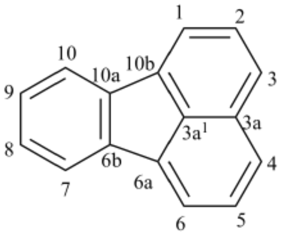
(7) pleiadene (PIN)


12
1
11
12a
2
10
10b
10a
9
3
4a
4b
4
8
5
6a
7
6

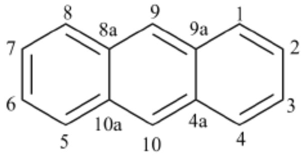
(8) chrysene (PIN)


10
1
9
10a
2
8a
3a1
3
8
5a1
3a
7
5a
4
6
5

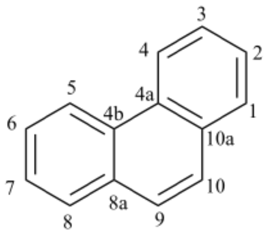
(9) pyrene (PIN)


1
2
10
10b
10a
3
9
3a1
3a
8
6b
4
7
6a
6
5

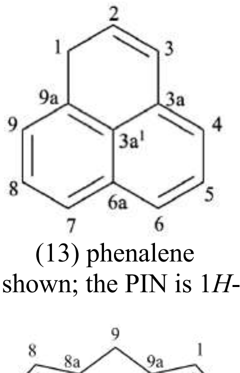
(10) fluoranthene (PIN)


8
9
1
8a
9a
7
2
6
3
10a
4a
5
10
4

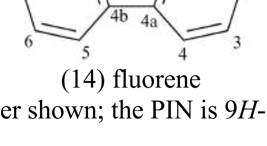
(11) anthracene (PIN)
(special numbering)


3
4
2
5
4a
6
4b
1
10a
7
10
8a
8
9

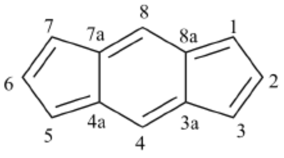
(12) phenanthrene (PIN)
(special numbering)


2
1
3
9a
3a
9
3a1
4
8
5
6a
7
6

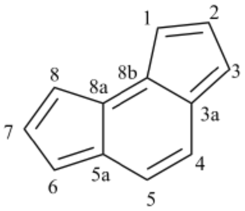
(13) phenalene
(1*H*-isomer shown; the PIN is 1*H*-phenalene)


9
8
8a
9a
1
7
2
4b
4a
6
5
4
3

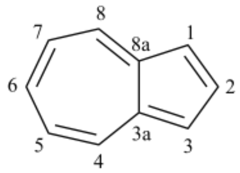
(14) fluorene
(9*H*-isomer shown; the PIN is 9*H*-fluorene)



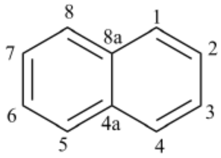
(15) *s*-indacene (PIN)



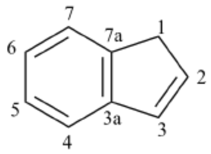
(16) *as*-indacene (PIN)



(17) azulene (PIN)



(18) naphthalene (PIN)



(19) indene
(1*H*-isomer shown; the PIN is 1*H*-indene)

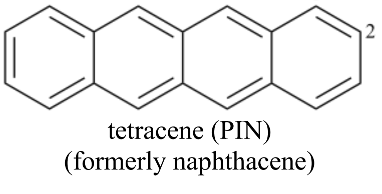
P-25.1.2 Systematically named hydrocarbon parent components

Names for some hydrocarbon parent components having the maximum number of noncumulative double bonds (called mancude ring systems) and having at least two rings of five or more ring members are systematically formed using a prefix and an ending or term representing the nature and arrangement of the component rings. Rules for numbering are described in Section P-25.3.3.

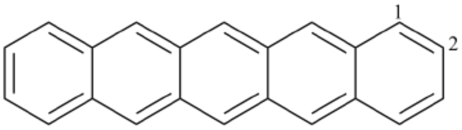
P-25.1.2.1 Polyacenes
P-25.1.2.2 Polyaphenes
P-25.1.2.3 Polyalenes
P-25.1.2.4 Polyphenylenes
P-25.1.2.5 Polynaphthylenes
P-25.1.2.6 Polyhelicenes
P-25.1.2.7 Ace...ylenes

P-25.1.2.1 Polyacenes. A hydrocarbon parent component consisting of four or more *ortho*-fused benzene rings in a straight linear arrangement is named by citing a numerical prefix (‘tetra’, ‘penta’, etc.) denoting the number of rings followed by the ending ‘acene’ (derived from the retained name anthr**acene**) with elision of a letter ‘a’.

Examples:

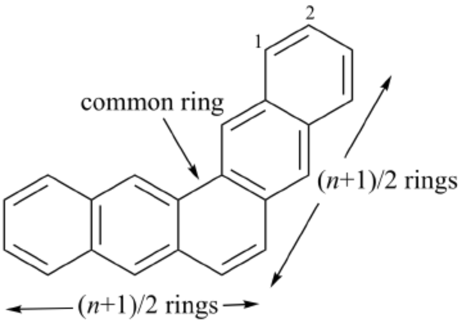


tetracene (PIN)
(formerly naphthacene)

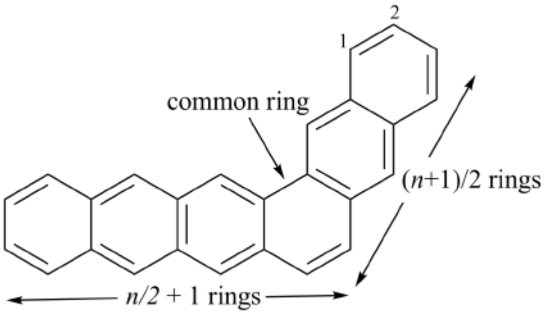


pentacene (PIN)

P-25.1.2.2 Polyaphenes. A hydrocarbon parent component consisting of *n* *ortho*- fused benzene rings ($n > 3$) forming two straight linear arrangements of $(n + 1)/2$ rings (if *n* is odd) or $n/2$ and $(n/2) + 1$ rings (if *n* is even) with a common benzene ring and that make a formal angle of 120° with each other is named by citing the numerical prefix ('tetra', 'penta', etc.) denoting the total number of benzene rings followed by the ending 'phene' (derived from **phen**anthrene).



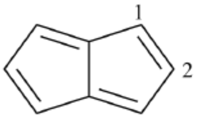
pentaphene ($n = 5$) (PIN)



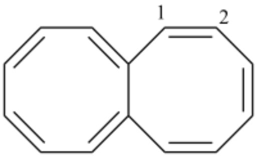
hexaphene ($n = 6$) (PIN)

P-25.1.2.3 Polyalenes. A hydrocarbon parent component consisting of two identical *ortho*-fused monocyclic hydrocarbon rings is named by citing the numerical prefix ('penta', 'hepta', etc.) that denotes the number of carbon atoms in each ring followed by the ending 'alene' (derived from naphth**alene**) with elision of a letter 'a'. The name naphthalene is retained.

Examples:



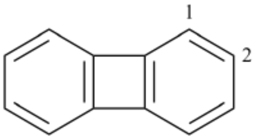
pentalene (PIN)



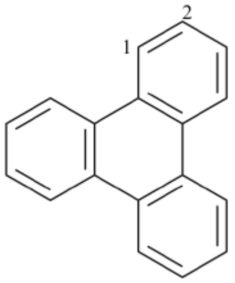
octalene (PIN)

P-25.1.2.4 Polyphenylenes. A hydrocarbon parent component consisting of a monocyclic hydrocarbon with an even number of carbon atoms and benzene rings *ortho*-fused to alternate sides is named by citing a numerical prefix ('tri', 'tetra', etc.) denoting the number of benzene rings followed by the term 'phenylene'. The traditional name biphenylene is retained.

Examples:



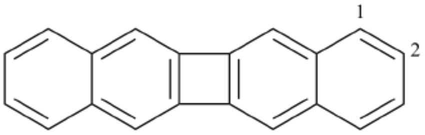
biphenylene (PIN)
(not diphenylene)



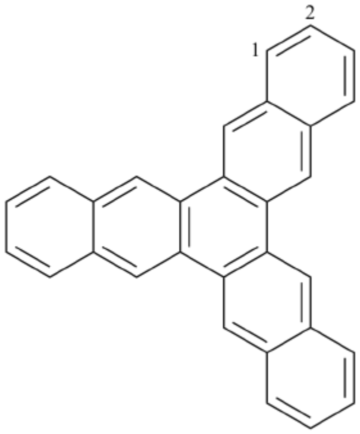
triphenylene (PIN)

P-25.1.2.5 Polynaphthylenes. A hydrocarbon parent component that consists of a monocyclic hydrocarbon with an even number of carbon atoms *ortho*-fused on alternate sides to the 2,3-positions of naphthalene rings is named by citing a numerical prefix ('tri', 'tetra', etc.) denoting the number of naphthalene rings followed by the term 'naphthylene'. The series begins with three naphthalene rings, trinaphthylene. The first member of the series, which would be dinaphthylene, is named as a fused hydrocarbon, i.e., dibenzo[*b*,*h*]biphenylene, and thus is not considered as a parent component.

Examples:



dibenzo[*b*,*h*]biphenylene (PIN)
(not dinaphthylene)

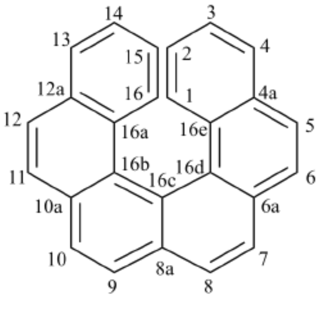


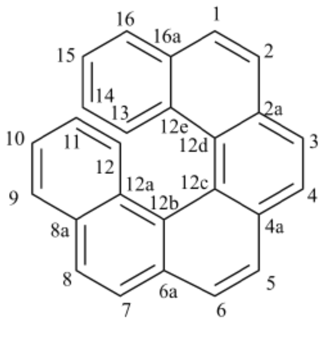
trinaphthylene (PIN)

P-25.1.2.6 Polyhelicenes. A hydrocarbon parent component of six or more rings that consists of a benzene ring *ortho*-fused to the 3,4-position of phenanthrene and further benzene rings fused in a similar way is named by citing a numerical prefix ('hexa', 'hepta', etc.) denoting the total number of benzene rings forming a helical arrangement followed by the term 'helicene'.

Note: The definition, orientation, and numbering of polyhelicenes was changed in the comprehensive fused ring nomenclature document 'Nomenclature of Fused and Bridged Fused Ring Systems' (ref. 4). The series begins with six rings and not five rings as indicated in the 1993 Guide (R-2.4.1.3.6 in ref. 2) and in the Glossary of Class Names (ref. 23). The new orientation and numbering are presented in Section P-25.3.3.1.1.

Example:



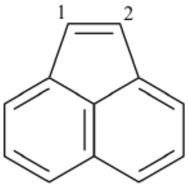


hexahelicene (PIN)
(new orientation and numbering)

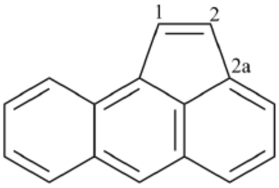
Note: Orientation and numbering no longer recommended; but still in use by CAS for the ring system having the name phenanthro[3,4-*c*]phenanthrene, ref. 22)

P-25.1.2.7 Ace....ylenes. A hydrocarbon parent component that consists of a five-membered ring *ortho*- and *peri*-fused to naphthalene, anthracene, or phenanthrene is named by adding the prefix ‘ace’ to the retained name and changing the ending ‘alene’, ‘acene’, or ‘ene’, respectively, to ‘ylene’.

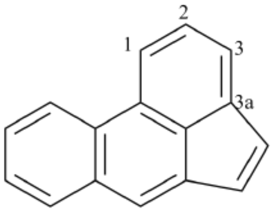
Examples:



acenaphthylene (PIN)



aceanthrylene (PIN)



acephenanthrylene (PIN)

P-25.2 NAMES OF HETEROCYCLIC PARENT RING COMPONENTS

P-25.2.1 Retained names used for parent components and as attached components
P-25.2.2 Names formed systematically using endings and prefixes used for parent components and attached components

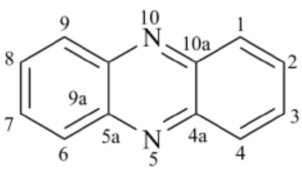
P-25.2.1 Retained names for heterocycles (also called trivial names) with the maximum number of noncumulative double bonds (called mancude ring systems) used for parent components and as attached components are given in Table 2.8.

Ring systems are arranged in decreasing order of seniority for parent compounds in accordance with the seniority order described in Section P-25.3.2.4 and exemplified in Section P-25.8.1.

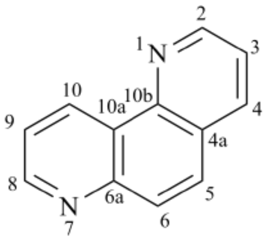
Skeletal replacement nomenclature, as described in Section P-15.5.2, is used to replace O by S, Se, and Te of chromene, isochromene, and xanthene (PIN) to generate names for chalcogen analogues of these ring systems (see Table 2.8). Some names listed in Table 2.8 can be modified by a system of replacement specific to some nitrogen-containing compounds, in which N is replaced by As or P. The modified names are listed in Table 2.9; the modifiable compounds are marked by the symbol * in Table 2.8. Rules for numbering are described in Section P-25.3.3.

Table 2.8 Retained names of heterocyclic parent ring components in descending order of seniority

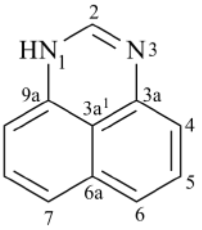
(the seniority order is indicated by the number preceding the name; the lower the number, the higher the seniority; names denoted by the symbol * are further modified as shown in Table 2.9)



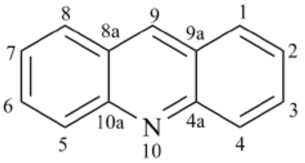
(1) phenazine (PIN)


2
1N
3
10
10a
10b
4
9
4a
8
N
6a
5
7
6

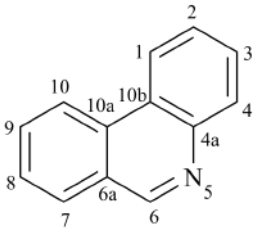
(2) phenanthroline
1,7-isomer shown; the PIN is 1,7-phenanthroline;
other isomers are: 1,8-; 1,9-; 1,10-; 2,7-; 2,8-; 2,9-; 3,7-; 3,8-; 4,7-)


2
HN
1
N3
9a
3a¹
3a
9
4
8
6a
5
7
6

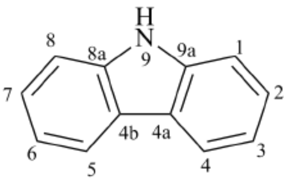
(3) perimidine (1*H*-isomer shown; the PIN is 1*H*-perimidine)


8
9
1
8a
9a
7
2
6
10a
N
4a
3
5
10
4

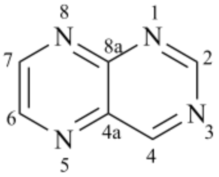
(4) acridine* (PIN)
(special numbering)


2
1
3
10
10a
10b
4
9
4a
8
6a
N
5
7
6

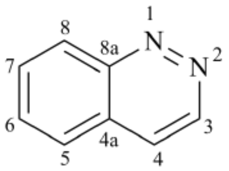
(5) phenanthridine* (PIN)


H
N
8
8a
9
9a
1
7
2
4b
4a
6
3
5
4

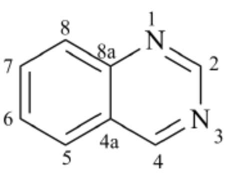
(6) carbazole
(special numbering; 9*H*-isomer shown; the PIN is 9*H*-carbazole)


8
1
N
8a
N
7
2
6
N
4a
N
3
5
4

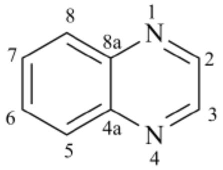
(7) pteridine (PIN)


1
8
8a
N
N
2
7
6
3
4a
5
4

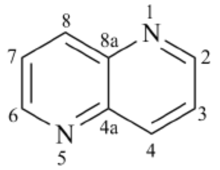
(8) cinnoline (PIN)


1
8
8a
N
7
2
6
N
3
4a
5
4

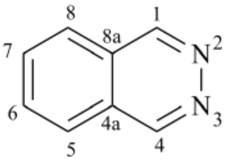
(9) quinazoline (PIN)


1
N
8
8a
2
7
3
6
4a
N
5
4

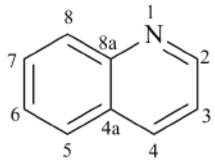
(10) quinoxaline (PIN)


1
N
8
8a
2
7
3
6
N
4a
5
4

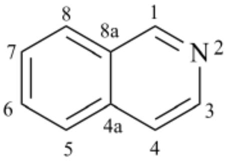
(11) naphthyridine
(1,5-isomer shown; the PIN is 1,5-naphthyridine;
other isomers are 1,6-; 1,7-; 1,8-; 2,6-; 2,7-)


8
1
8a
N 2
7
N 3
6
4a
5
4

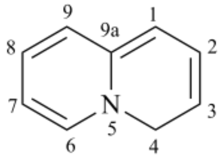
(12) phthalazine (PIN)


1
N
8
8a
2
7
3
6
4a
5
4

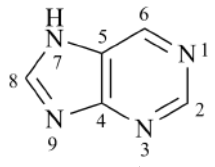
(13) quinoline*† (PIN)


8
1
8a
N 2
7
3
6
4a
5
4

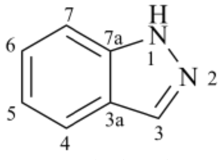
(14) isoquinoline*† (PIN)


9
1
9a
8
2
7
N
3
5
6
4

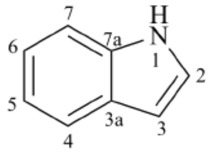
(15) quinolizine*†
(4*H*-isomer shown; the PIN is 4*H*-quinolizine)


H
N
6
5
7
N 1
8
2
N
4
N
9
3

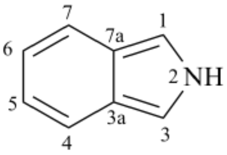
(16) purine
(special numbering, 7*H*-isomer shown; the PIN is 7*H*-purine)


7
H
N
6
7a
1
N 2
5
3a
3
4

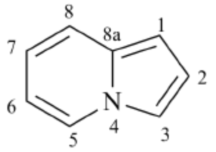
(17) indazole
(1*H*-isomer shown; the PIN is 1*H*-indazole)



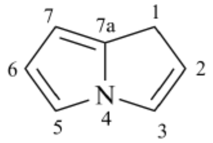
(18) indole*
(1*H*-isomer shown; the PIN is 1*H*-indole)



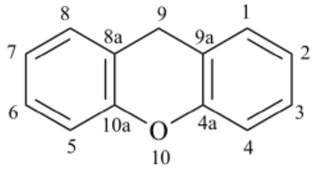
(19) isoindole*
(2*H*-isomer shown; the PIN is 2*H*-isoindole)



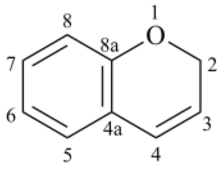
(20) indolizine* (PIN)



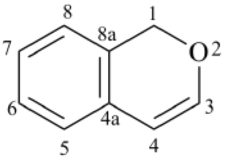
(21) pyrrolizine (1*H*-isomer shown; the PIN is 1*H*-pyrrolizine)



(22) xanthene
(special numbering; 9*H*-isomer shown; the PIN is 9*H*-xanthene)
thioxanthene (S instead of O)
(special numbering; 9*H*-isomer shown; the PIN is 9*H*-thioxanthene)
selenoxanthene (Se instead of O)
(special numbering; 9*H*-isomer shown; the PIN is 9*H*-selenoxanthene)
telluroxanthene (Te instead of O)
(special numbering; 9*H*-isomer shown; the PIN is 9*H*-telluroxanthene)



(23) chromene
(2*H*-isomer shown)
1-benzopyran
(2*H*-isomer shown; the PIN is 2*H*-1-benzopyran)
thiochromene (S instead of O)
(2*H*-isomer shown)
1-benzothiopyran (S instead of O)
(2*H*-isomer shown; the PIN is 2*H*-1-benzothiopyran
selenochromene (Se instead of O)
(2*H*-isomer shown)
1-benzoselenopyran (Se instead of O)
(2*H*-isomer shown; the PIN is 2*H*-1-benzoselenopyran)
tellurochromene (Te instead of O)
(2*H*-isomer shown)
1-benzotelluropyran (Te instead of O)
(2*H*-isomer shown; the PIN is 2*H*-1-benzotelluropyran)



(24) isochromene
(1*H*-isomer shown)

2-benzopyran
(1*H*-isomer shown; the PIN is 1*H*-2-benzopyran)

isothiochromene (S instead of O)
(1*H*-isomer shown)

2-benzothiopyran (S instead of O)
(1*H*-isomer shown; the PIN is 1*H*-2-benzothiopyran)

isoselenochromene (Se instead of O)
(1*H*-isomer shown)

2-benzoselenopyran (Se instead of O)
(1*H*-isomer shown; the PIN is 1*H*-2-benzoselenopyran)

isotellurochromene (Te instead of O)
(1*H*-isomer shown)

2-benzotelluropyran (Te instead of O)
(1*H*-isomer shown; the PIN is 1*H*-2-benzotelluropyran)

† In CAS index nomenclature, quinolizine precedes quinoline and isoquinoline in seniority.

Table 2.9 Names for nitrogenous parent components modified by phosphorus and arsenic replacement
(For the seniority of the phosphorus and arsenic ring systems see P-25.3.2.4 and P-25.8.1)
In the following names, arsenic or phosphorus atoms replace nitrogen atoms

Nitrogen ring system	Arsenic ring system	Phosphorus ring system
acridine (PIN)	acridarsine (PIN)*	acridophosphine (PIN)*
indole (PIN)	arsindole (PIN)	phosphindole (PIN)
indolizine (PIN)	arsindolizine (PIN)	phosphindolizine (PIN)
isoindole (PIN)	isoarsindole (PIN)	isophosphindole (PIN)
isoquinoline (PIN) †	isoarsinoline (PIN)	isophosphinoline (PIN)
phenanthridine (PIN)	arsanthridine (PIN)	phosphanthridine (PIN)
quinoline (PIN) †	arsinoline (PIN)	phosphinoline (PIN)
quinolizine (PIN) †	rsinolizine (PIN)	phosphinolizine (PIN)

* Numbered systematically, not as acridine.

† In CAS index nomenclature, quinolizine precedes quinoline and isoquinoline in seniority.

P-25.2.2 Systematically named heterocyclic components

P-25.2.2.1 Heteromonocyclic parent components
P-25.2.2.2 Heteranthrene components
P-25.2.2.3 Pheno...ine components
P-25.2.2.4 Heteromonocyclic components fused to a benzene ring

P-25.2.2.1 Heteromonocyclic parent components

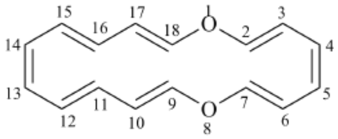
P-25.2.2.1.1 Heteromonocyclic rings with three through ten ring members having the maximum number of noncumulative double bonds (called mancude ring systems) are used as parent components as well as attached components. Retained names are given in Table 2.2. Hantzsch-Widman names are discussed in P-22.2.2.

P-25.2.2.1.2 Names of heteromonocyclic parent components with more than ten ring members used in fusion nomenclature are discussed in this subsection; they are used only in fusion nomenclature (see also P-22.2.4). The preferred IUPAC names for such rings are 'polyene' names (see P-22.2.4).

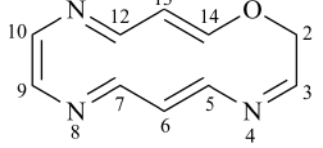
A heteromonocyclic parent component having more than ten members and the maximum number of noncumulative double bonds (a mancude ring system) may be named by changing the ending 'ane' of the corresponding saturated heteromonocycle (see P-22.2.4) to 'ine'. Their locants are cited in front of the name following indicated hydrogen, if any, in the order of the appearance of the corresponding replacement ('a') prefixes in the name.

For examples of fusion compounds including this type of heteromonocyclic parent component, see P-25.2.2.4.

Examples:



1,8-dioxacyclooctadecine
1,8-dioxacyclooctadeca-2,4,6,9,11,13,15,17-octaene (PIN)

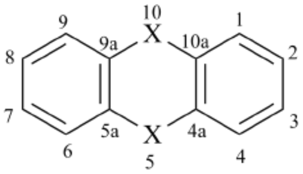


2*H*-1,4,8,11-oxatriazacyclotetradecine
1-oxa-4,8,11-triazacyclotetradeca-3,5,7,9,11,13-hexaene (PIN)

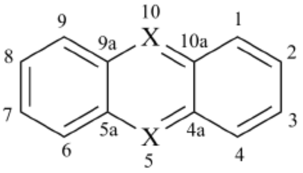
P-25.2.2.2 Heteranthrene components

A heterotricyclic parent component consisting of two benzene rings fused to a 1,4-dihetera-benzene in which the heteroatoms are the same is named by attaching the appropriate 'a' prefix to the ending 'anthrene' (derived from anthracene), with elision of a letter 'a'. The allowed heteroatoms are O, S, Se, Te, P, As, Si, and B. When the heteroatoms are nitrogen atoms, the component is named 'phenazine' (a retained name). The numbering is standard, as shown. Rules for numbering are described in Section P-25.3.3.

Examples:



X = O oxanthrene (PIN)
X = S thianthrene (PIN)
X = Se selenanthrene (PIN)
X = Te telluranthrene (PIN)

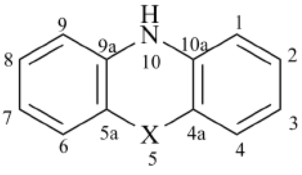


X = N phenazine (PIN)
(a retained name)
X = P phosphanthrene (PIN)
X = As arsanthrene (PIN)
X = B boranthrene (PIN)
X = SiH silanthrene (PIN)

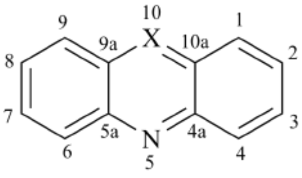
P-25.2.2.3 Pheno...ine components

A heterotricyclic parent component consisting of two benzene rings fused to a 1,4-dihetera-benzene in which the heteroatoms are different is named by adding the prefix 'pheno' (derived from **phen**anthrene) to the appropriate Hantzsch-Widman name (see P- 22.2.2), eliding the 'o' before a following vowel. Numbering is standard and depends on the nature of the heteroatoms. Rules for numbering are described in Section P-25.3.3.

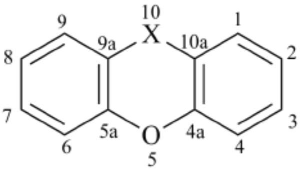
Examples:



X = O phenoxazine (10*H*-isomer shown; the PIN is 10*H*-phenoxazine)
X = S phenothiazine (10*H*-isomer shown; the PIN is 10*H*-phenothiazine)
X = Se phenoselenazine (10*H*-isomer shown; the PIN is 10*H*-phenoselenazine)
X = Te phenotellurazine (10*H*-isomer shown; the PIN is 10*H*-phenotellurazine)



X = P phenazaphosphinine (PIN)
phenophosphazine (see refs. 2, 4)
X = As phenazarsinine (PIN)
phenarsazine (see refs. 2, 4)



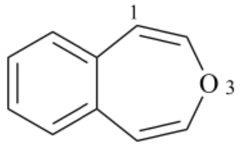
X = S phenoxathiine (PIN)
X = Se phenoxaselenine (PIN)
X = Te phenoxatellurine (PIN)
X = PH phenoxaphosphinine (PIN, 10*H*-isomer shown)
phenoxaphosphine (10*H*-isomer shown)
X = AsH phenoxarsinine (PIN, 10*H*-isomer shown)
phenoxarsine (10*H*-isomer shown)
X = SbH phenoxastibinine (PIN, 10*H*-isomer shown)
phenoxantimonine (10*H*-isomer shown)
X = AsH; and S instead of O phenothiarsinine (PIN, 10*H*-isomer shown)
phenothiarsine (10*H*-isomer shown)

P-25.2.2.4 Heteromonocyclic components fused to a benzene ring

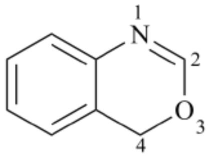
If the initial identified preferred components for naming a fused ring system include an isolated benzo component (i.e. not forming part of a component with a retained name such as quinoline or anthracene) *ortho*-fused to a heteromonocyclic component of five or more members, these two components are treated together as a one-component unit (a benzoheterocycle). See P-25.3.5 for the use of benzoheterocycles in fusion nomenclature and limitations on its use. It is named by placing the locant(s) indicating the position(s) of the heteroatom(s) at the front of the name consisting of the fusion prefix 'benzo' followed by a retained name, a Hantzsch-Widman systematic name, or a name formed by skeletal replacement ('a') nomenclature as described in P-25.2.2.1.2. The locants cited correspond to the full bicyclic structure. As in Hantzsch-Widman names, locants are placed in the order corresponding to the order of citation of the heteroatoms in the heterocyclic component. The locant '1' is always assigned to the atom of the heterocyclic component next to a fusion atom. Heteroatoms are allocated lowest locants as a set, without regard to kind; if there is a choice, lowest locants are assigned in accordance with the seniority of the 'a' prefixes (see Table 2.4). In general nomenclature locants may be omitted when the name is unambiguous; for preferred IUPAC names locants must be cited. The letter 'o' of the 'benzo' prefix is elided when followed by a vowel. Indicated hydrogen is placed at the front of the name, when required.

'Benzo names' offer several advantages. They are simpler in the sense that they do not require fusion descriptors. However, their primary advantage is in their use as components of fusion names; they provide a larger portion of structure and remove one full level of locants in the construction of names for larger heterocyclic fused ring systems.

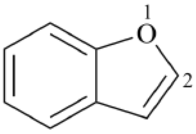
Examples:



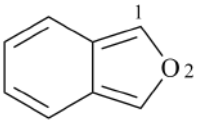
3-benzoxepine (PIN)
benzo[*d*]oxepine



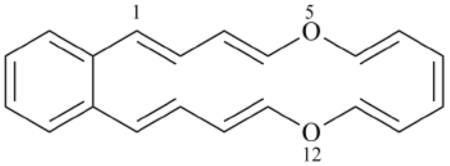
4*H*-3,1-benzoxazine (PIN)
4*H*-benzo[*d*][1,3]oxazine



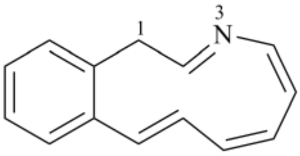
1-benzofuran (PIN)
benzofuran



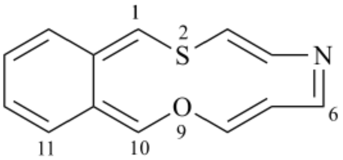
2-benzofuran (PIN)
isobenzofuran
benzo[*c*]furan



5,12-benzodioxacyclooctadecine (PIN)
benzo[*m*][1,8]dioxacyclooctadecine



1*H*-3-benzazacycloundecine (PIN)
1*H*-benzo[*h*][1]azacycloundecine
1*H*-3-benzoazacycloundecine



9,2,5-benzoxathiaazacyclododecine (PIN)
(not 2,9,6-benzoxathiaazacyclododecine; the locant set 2,5,9 is lower than 2,6,9)
benzo[*j*][1,8,5]oxathiaazacyclododecine

P-25.3 CONSTRUCTING FUSION NAMES

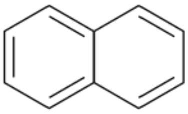
- P-25.3.1 Definitions, terminology, and general principles
- P-25.3.2 Constructing two-component fusion names
- P-25.3.3 Numbering of fused ring systems
- P-25.3.4 Constructing polycomponent fusion names
- P-25.3.5 Heteromonocyclics fused to a benzene ring
- P-25.3.6 Identical attached components
- P-25.3.7 Multiparent ring systems
- P-25.3.8 Omission of locants in fusion descriptors

P-25.3.1 Definitions, terminology, and general principles

P-25.3.1.1 Definitions

P-25.3.1.1.1 *ortho*-Fused. Two rings that have only two atoms and one bond in common are said to be *ortho*-fused

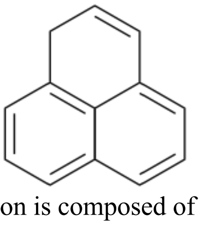
Example:



The two benzene rings of the naphthalene skeletal ring system are *ortho*-fused.

P-25.3.1.1.2 *ortho*- and *peri*-Fused. In a polycyclic compound a ring ortho-fused to different sides of two other rings that are themselves *ortho*-fused together (i.e. there are three common atoms between the first ring and the other two) is said to be *ortho*- and *peri*-fused to the other two rings.

Example:



The phenylene skeleton is composed of three benzene rings,
each *ortho*- and *peri*-fused to the other two

P-25.3.1.1.3 Fusion atom. Any atom of a fused ring system that is common to two or more rings.

P-25.3.1.1.4 Peripheral atom. Any atom that forms part of the outer perimeter of a fused ring system.

P-25.3.1.1.5 Interior atom. Any fusion atom that is not peripheral.

P-25.3.1.2 Terminology

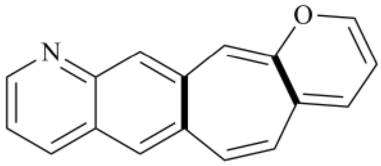
P-25.3.1.2.1 Components of a fused ring system. Fusion components are mancude or ring systems that can be named without the application of any fusion nomenclature principles. Fused ring systems that do not have such a name are named by joining together the names of appropriately selected fusion components.

P-25.3.1.2.2 Parent component. The parent component according to the terminology of the 1998 recommendations (ref. 4) (referred to as base component in the 1979 publication, ref. 1; and principal component in the 1993 Recommendations, ref. 2) is the one with highest seniority according to the criteria given in P-25.3.2.4. A parent component may be mono- or polycyclic, but it must be a mancude ring or ring system. Its name is never modified and is cited last in the name of the fused system.

P-25.3.1.2.3 Attached component

. The components of a fused ring system not included in the parent component are called attached components. The attached components are called first-order, second-order, etc. attached components when they correspond to the first, second, etc. attached component reached when moving away from the parent component across fusion sites. An attached component may be mono- or polycyclic, but it must be a mancude ring or ring system. Fusion sites are bold lines in the following examples.

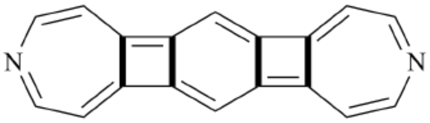
Example:



Explanation: The bicyclic component at the left end of the above structure is the parent component, the seven-membered ring fused to the parent component is the first-order attached component; the six-membered ring fused to the first-order attached component is the second-order attached component.

P-25.3.1.2.4 Interparent components. In a system that consists of two (or more) parent components *ortho*- or *ortho*- and *peri*-fused to the same attached component, the latter is called an interparent component. Likewise, if two (or more) parent components are fused to three or more appropriately attached components, there will be two first- order interparent components and a second-order interparent component. Fourth-, fifth-, etc. order components may be present in more complex systems.

Example:



Explanation: The two seven-membered rings are the parent components; the two four-membered rings are the first order interparent components; the six-membered ring is the second-order interparent component.

P-25.3.1.3 General principles

‘*ortho*-Fused’ or ‘*ortho*- and *peri*-fused’ polycyclic ring systems with the maximum number of noncumulative double bonds (mancude) that have no accepted retained or systematic name described in sections P-25.1 and P-25.2 are named by prefixing to the name of a component ring or ring system (the parent component) designations of the other component(s) (attached components). For fused ring systems in preferred IUPAC names, see P-52.2.4.

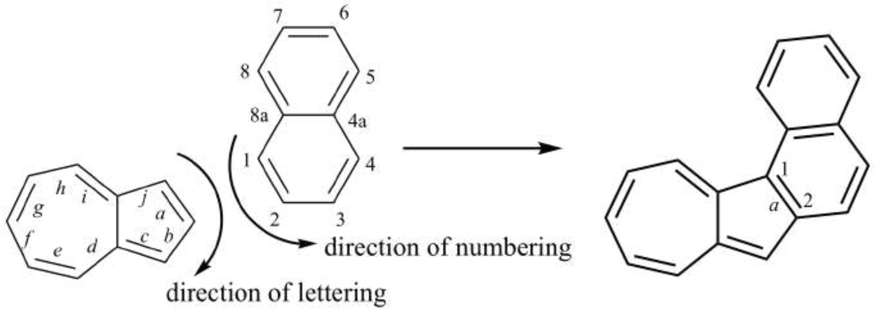
The parent component is selected by applying criteria of seniority as described in P- 25.3.2.4 below. In a fusion name, the name of the parent component is that of the component itself. The names of attached components are formed by replacing the last letter ‘e’ by ‘o’ in the name of the component, i.e., indeno from indene (or by adding the letter ‘o’ when no final letter ‘e’ is present, i.e., pyrano from pyran) or by other means described in P-25.3.2.2 below. There is no elision of the final letter ‘o’ or ‘a’ before a vowel (see Rule FR-4.7, ref. 4).

Locants that describe structural features of components, such as positions of heteroatoms, are kept with the name of the component and are enclosed within square brackets.

Note: In preferred IUPAC names the elision of the final letter ‘o’ of ‘acenaphtho’, ‘benzo’, ‘naphtho’ and ‘perylo’ and the final letter ‘a’ of the monocyclic prefixes ‘cyclopropa’, ‘cyclobuta’, etc. is not recommended as indicated in FR-4.7 of the 1998 publication, ref. 4; hence, ‘benzo[*g*]isoquinoline’ rather than ‘benz[*g*]isoquinoline’. However this elision as recommended in the 1979 recommendations (Rule A-21.4, ref. 1) may be continued in general nomenclature.

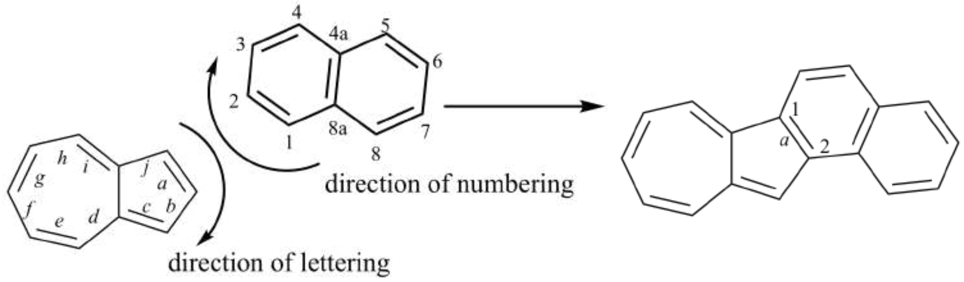
Isomers are distinguished by lettering, continuously, each peripheral side of the parent component (including sides whose locants are distinguished by letters, for example, 2a,3a) using the italic letters *a*, *b*, *c*, etc., beginning with *a* for the side numbered ‘1,2’, *b* for ‘2,3’ etc.. To the letter as early in the alphabet as possible that denotes the side where the fusion occurs are prefixed, if necessary, the numbers of the positions of attachment of the other component. These numbers are chosen to be as low as is consistent with the numbering of the compound and their order conforms to the direction of lettering of the parent component. In this document these letters and numbers are placed within the structure of the ring or ring system.

Examples:


7
6
8
5
8a
4a
1
4
2
3
h
i
j
g
a
f
e
d
c
b
direction of numbering
direction of lettering
1
a
2

azulene (PIN) + naphthalene (PIN)
(parent component) (attached component)

naphtho[1,2-*a*]azulene (PIN)

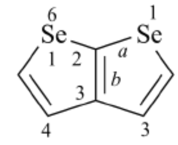

4
4a
5
3
6
2
1
8a
7
8
h
i
j
g
a
f
e
d
c
b
direction of numbering
direction of lettering
1
a
2

azulene (PIN) + naphthalene (PIN)
(parent component) (attached component)

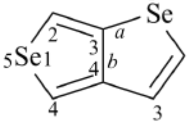
naphtho[2,1-*a*]azulene (PIN)

The numbers and letters, separated by commas when required, are enclosed in square brackets and placed immediately after the designation of the attached component; there is no space or hyphen either preceding or following the brackets. Hyphens separate the two parts of a fusion descriptor, i.e., numbers and italicized letters. This expression merely defines the manner of fusion of the components. Indicated hydrogen atoms are added to the names, as required, using locants characterizing the fused system.

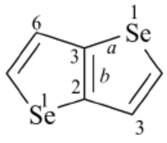
Examples:


6
Se
1
Se
1
2
a
b
3
4
3

selenopheno[2,3-*b*]selenophene (PIN)


1
Se
2
3
a
5Se1
4
b
4
3

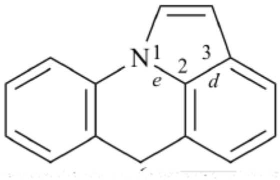
selenopheno[3,4-*b*]selenophene (PIN)


1
6
Se
3
a
2
b
1
Se
3

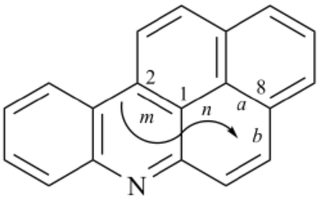
selenopheno[3,2-*b*]selenophene (PIN)

ortho- and *peri*-Fused ring systems require a fusion descriptor that indicates all fused bonds. All letters referring to the parent component are cited, but only locants of the nonfused atoms of the attached component are indicated. Letters are not separated by commas in the fusion descriptor.

Examples:



6*H*-pyrrolo[3,2,1-*de*]acridine



naphtho[2,1,8-*mna*]acridine

P-25.3.2 Constructing two-component fusion names

A component may be monocyclic or polycyclic. Systematic construction proceeds stepwise as follows.

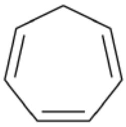
P-25.3.2.1 Selecting and naming parent components for fusion nomenclature
P-25.3.2.2 Prefixes for attached components
P-25.3.2.3 Orientation of fused ring systems
P-25.3.2.4 Seniority criteria for selecting parent components
P-25.3.2.5 Assembling components and naming fused ring systems

P-25.3.2.1 Selecting and naming parent components for fusion nomenclature

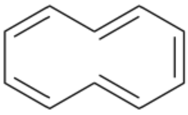
P-25.3.2.1.1 Monocyclic hydrocarbons (annulenes).

Monocyclic parent components are named as [*n*]annulenes where n represent the number of carbon atoms. The series starts at *n* = 7, because the retained name ‘benzene’ is preferred for *n* = 6. The use of the name ‘annulene’ in fusion nomenclature was recommended in the 1993 Guide (see R-2.3.1.2, ref. 2) to obviate the potential ambiguity of using contracted traditional names, such as cycloheptene to denote 1,3,5-cycloheptatriene.

Examples:



1*H*-[7]annulene
(no longer cycloheptene as fusion component)
cyclohepta-1,3,5-triene (PIN)



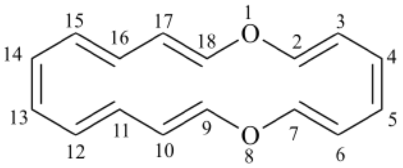
[10]annulene
(no longer cyclodecene as fusion component)
cyclodeca-1,3,5,7,9-pentaene (PIN)

P-25.3.2.1.2 Heteromonocycles

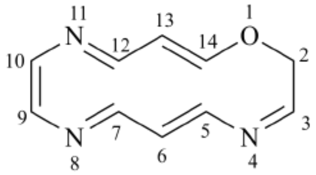
The retained names given in Table 2.2, except for ‘isothiazole’, ‘isoxazole’, ‘thiazole’, and ‘oxazole’, and Hantzsch-Widman names for unsaturated heteromonocycles (see P-22.2.2) are used as parent components in fusion nomenclature. The names ‘isothiazole’, ‘isoxazole’, ‘thiazole’, and ‘oxazole’, although permitted in general nomenclature, are not recommended for the names of components in preferred IUPAC fusion names. The Hantzsch-Widman names 1,2-thiazole, 1,2-oxazole, 1,3- thiazole, and 1,3-oxazole, respectively, must be used; the locants are enclosed in square brackets in the completed fusion name.

Heteromonocycles having more than ten members and the maximum number of noncumulative double bonds whose names are denoted by the ‘ine’ ending described in P-25.2.2.1.2 are used as parent components in preferred IUPAC fusion names.

Examples:



1,8-dioxacyclooctadecine
1,8-dioxacyclooctadeca-2,4,6,9,11,13,15,17-octaene (PIN)



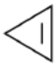
2*H*-1,4,8,11-oxatriazacyclotetradecine
1-oxa-4,8,11-triazacyclotetradeca-3,5,7,9,11,13-hexaene (PIN)

P-25.3.2.1.3 Names of the hydrocarbons and heterocycles described in Sections P-25.1.2 and P-25.2.2 and retained names listed in Tables 2.2, 2.7, and 2.8 are used as parent components for preferred IUPAC fusion names.

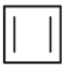
P-25.3.2.2 Prefixes for attached components.

P-25.3.2.2.1 Monocyclic hydrocarbon prefixes for attached components other than ‘benzo’ are formed by dropping ‘ne’ from the name of the appropriate saturated monocyclic hydrocarbon. These names represent the form with the maximum number of noncumulative double bonds. There is no upper ring-size limit to this criterion.

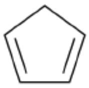
Examples:



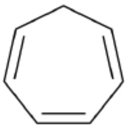
cyclopropa (preferred prefix)
(from cyclopropane, PIN)



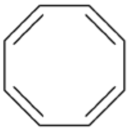
cyclobuta (preferred prefix)
(from cyclobutane, PIN)



cyclopenta (preferred prefix)
(from cyclopentane, PIN)



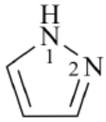
cyclohepta (preferred prefix)
(from cycloheptane, PIN)
(not [7]annuleno)



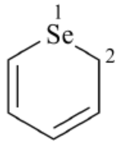
cycloocta (preferred prefix)
(from cyclooctane, PIN)
(not [8]annuleno)

P-25.3.2.2.2 Prefixes for attached components derived from the name of a parent component described in P-25.3.2.1.2 and P-25.3.2.1.3 are named by changing the final letter ‘e’ into the letter ‘o’ or by adding the letter ‘o’ when no final letter ‘e’ is present.

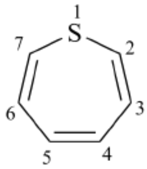
Examples:



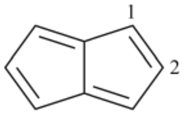
pyrazolo (preferred prefix)
(from pyrazole, PIN)



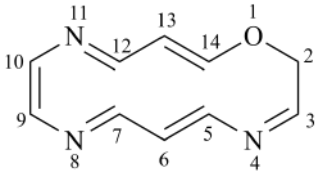
selenopyrano (preferred prefix)
(from selenopyran, PIN)



thiepino (preferred prefix)
(from thiepine, PIN)



pentaleno (preferred prefix)
(from pentalene, PIN)



1,4,8,11-oxatriazacyclotetradecino (preferred prefix)
(from 1,4,8,11-oxatriazacyclotetradecine, see P-25.2.2.1.2, P-25.3.2.1.2)

P-25.3.2.2.3 Retained prefixes

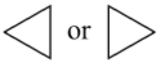
Only the following contracted prefixes are retained for preferred IUPAC fusion names. The contracted prefixes acenaphtho, perylo, isoquino, and quino are retained but are only used in general nomenclature.

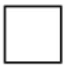
anthra (preferred prefix) (from anthracene, PIN)
naphtho (preferred prefix) (from naphthalene, PIN)
benzo (preferred prefix) (from benzene, PIN)
phenanthro (preferred prefix) (from phenanthrene, PIN)
furo (preferred prefix) (from furan, PIN)
imidazo (preferred prefix) (from imidazole, PIN)
pyrido (preferred prefix) (from pyridine, PIN)
pyrimido (preferred prefix) (from pyrimidine, PIN)
thieno (preferred prefix) (from thiophene (PIN)

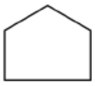
P-25.3.2.3 Orientation of fused ring systems

P-25.3.2.3.1 Drawing of ring structures

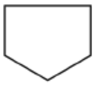
For the purpose of selecting parent components and for numbering of fused ring systems, the structures of fused ring compounds must be drawn in a specific manner according to a set of criteria that must be applied in order until a decision is reached. Individual rings of a polycyclic '*ortho*-fused' or '*ortho*- and *peri*-fused' hydrocarbon ring system are drawn in such a way so that as many as possible of the various individual rings are arranged in horizontal rows. If the compound requires distorted rings not shown above see P-25.3.2.2. Such rows are characterized by a horizontal axis that divides each individual ring into two approximate halves. Permitted shapes for three- to eight-membered rings are as follows:

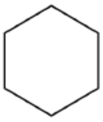


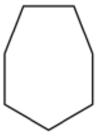




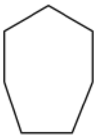
or

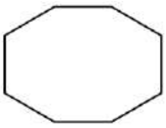


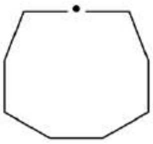




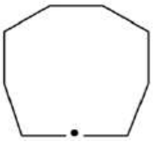
or



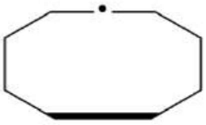




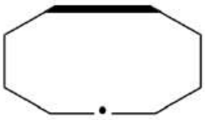
or



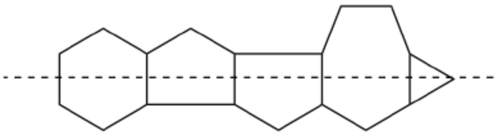
or



or



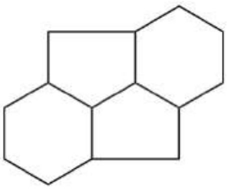
Example:



a horizontal row and its horizontal axis

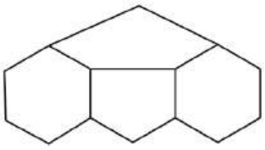
P-25.3.2.3.2 Distorted ring shapes

If a compound cannot be drawn only using the shapes shown in P-25.3.2.3.1 a distorted ring shape will be required. The distorted ring should be as small as possible.

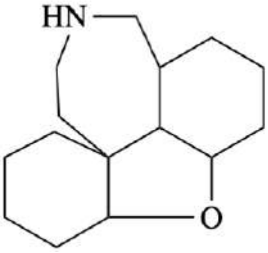


only preferred shapes used

not

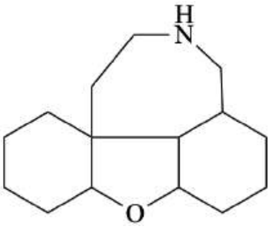


distorted five-membered ring

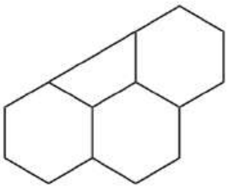


only preferred shapes used
(the separation to show the
seven-membered is not fused to
the left hand ring does not
count as distortion

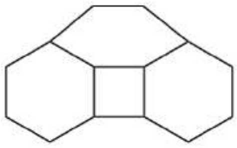
not



distorted seven-membered ring



not



distorted four-membered ring distorted six-membered ring

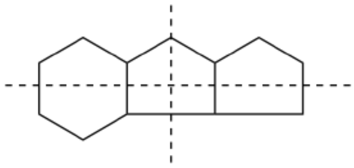
P-25.3.2.3.3 Criteria for selection of the preferred orientation

Polycyclic fused ring systems are oriented in accordance with the following criteria considered in order until a decision is reached:

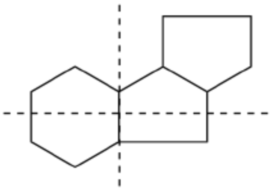
(a) maximum number of rings in a horizontal row;

Fused ring systems are drawn in order to achieve the maximum number of *ortho*-fused rings, with vertical common bonds, in a horizontal row. The relevant vertical bonds are always those furthest apart. If the correct orientation is not immediately apparent the horizontal row is bisected by a horizontal axis and a vertical axis to form four quadrants. Rings, which are not bisected by the horizontal axis, do not belong to the main row and are not considered in the counting of rings in the main row.

Examples:



3 rings in horizontal row



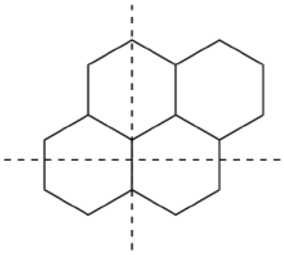
2 rings in horizontal row

Accordingly, polyacenes are senior to polyaphenes for an equal number of rings, and anthracene is senior to phenanthrene

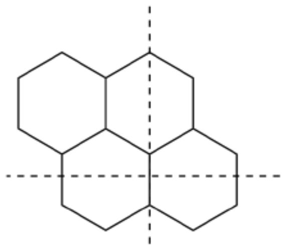
(b) maximum number of rings in upper right quadrant;

In the preferred orientation, the maximum number of rings must appear above and to the right of the horizontal row (upper right quadrant). For this purpose, the center of the horizontal row is defined as the central common bond if there is an even number of rings in the row, and the center of the central ring if there is an odd number of rings. In counting rings in a quadrant those rings that are divided by an axis are considered as two halves, and a ring bisected by both axes, counts as four quarters (one in each quadrant). Rings that are bisected by the horizontal axis but are not directly *ortho*-fused to the main row are not considered when counting how many rings are in the horizontal row.

Examples:

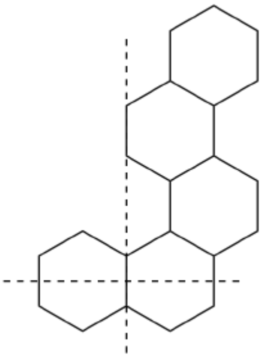


not



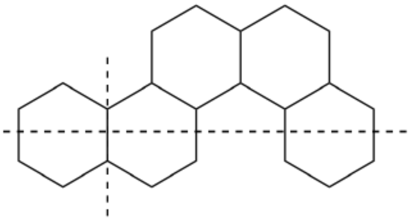
(correct orientation)
2 rings in horizontal row
2 rings in upper right quadrant

(incorrect orientation)
2 rings in horizontal row
1 ring in upper right quadrant



(correct orientation)
2 rings in the horizontal row
3½ rings in upper right quadrant

not

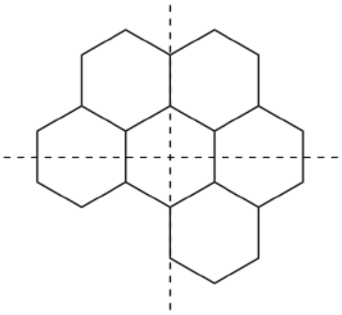


(incorrect orientation)
2 (not 3) rings in the horizontal row
3 rings in upper right quadrant

Accordingly, phenanthrene (1½ rings in the upper right quadrant) is senior to phenalene [1 ring (two ½ rings) in the upper right quadrant].

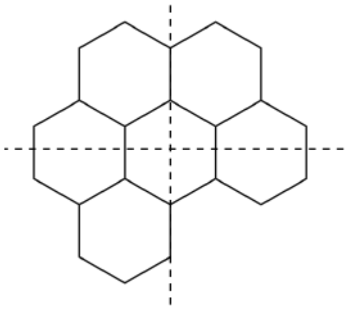
(c) minimum number of rings in the lower left quadrant;

Example:



(correct orientation)
3 rings in horizontal row
1¾ rings in upper right quadrant
¾ ring in lower left quadrant

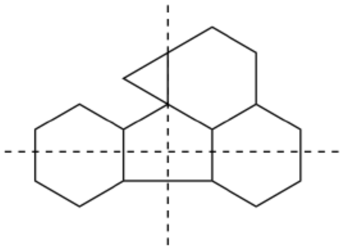
not



(incorrect orientation)
3 rings in horizontal row
1¾ ring in upper right quadrant
1¾ ring in lower left quadrant

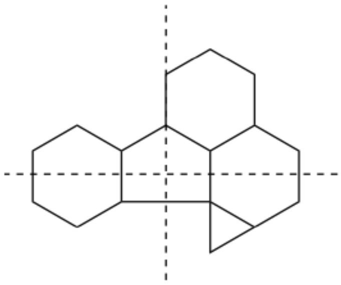
(d) maximum number of rings above the horizontal row.

Examples:



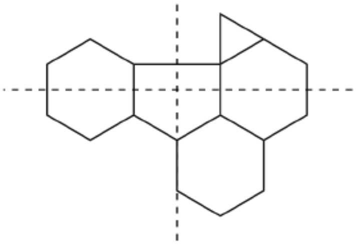
(correct orientation)
3 rings in horizontal row
1¾ rings in upper right quadrant
¾ ring in lower left quadrant
3½ rings above horizontal row

not



(incorrect orientation)
3 rings in horizontal row
1¾ ring in upper right quadrant
¾ ring in lower left quadrant
2½ rings above horizontal row

not



(incorrect orientation)
3 rings in horizontal row
1¾ ring in upper right quadrant
¾ ring in lower left quadrant
2½ rings above horizontal row

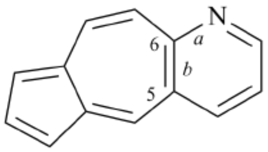
P-25.3.2.4 Seniority criteria for selecting the parent component

The components of the fused ring system are selected and named according to P-25.3.2.1 and P-25.3.2.2. When it is necessary to locate nomenclatural features, such as indicated hydrogen or atoms with nonstandard bonding numbers, another system of locants must be used, i.e., the locants that are used to number the completed fused ring system. In these recommendations, such locants are placed outside the structure, as shown for retained names in Tables 2.2, 2.7, and 2.8. This system is fully explained and exemplified in P-25.3.3.

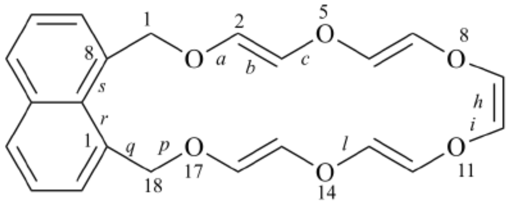
If there is a choice for selecting the parent component, the following criteria are considered, in order, until a decision can be made:

(a) a component containing at least one of the heteroatoms occurring earlier in the following order: N > F > Cl > Br > I > O > S > Se > Te > P > As > Sb > Bi > Si > Ge > Sn > Pb > B > Al > Ga > In > Tl;

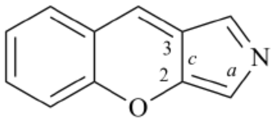
Examples:



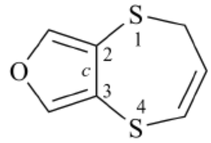
azuleno[6,5-*b*]pyridine (PIN)
[pyridine (heterocycle) is senior to azulene (carbocycle)]



1*H*,18*H*-naphtho[1,8-*rs*][1,4,7,10,13,16]hexaoxacyclohenicosine (PIN)
[1,4,7,10,13,16-hexaoxacyclohenicosine (heterocycle) is senior to naphthalene (carbocycle)]



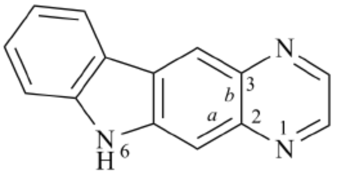
[1]benzopyrano[2,3-*c*]pyrrole (PIN)
(pyrrole is senior to 1-benzopyran N > O)
chromeno[2,3-c]pyrrole



2*H*-[1,4]dithiepino[2,3-*c*]furan (PIN)
(furan is senior to dithiepine; O > S)

(b) a component containing the greater number of rings;

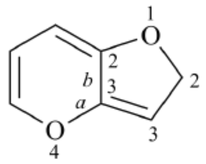
Example:



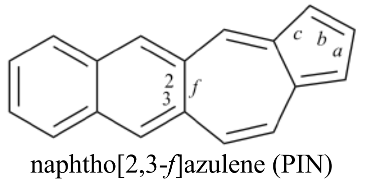
6*H*-pyrazino[2,3-*b*]carbazole (PIN)
[carbazole (3 rings) is senior to quinoxaline (2 rings)]

(c) A component containing the larger ring at the first point of difference when comparing rings in order of decreasing size;

Examples



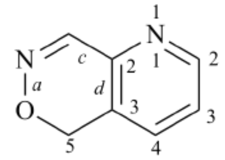
2*H*-furo[3,2-*b*]pyran (PIN)
[pyran (6 ring) preferred to furan (5 ring)]



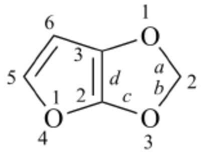
naphtho[2,3-*f*]azulene (PIN)
[azulene (7,5 rings) preferred to naphthalene 6,6 rings)]

(d) A component containing the greater number of heteroatoms of any kind;

Examples:



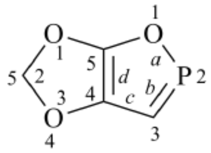
5*H*-pyrido[2,3-*d*][1,2]oxazine (PIN)
[oxazine (2 heteroatoms) preferred to pyridine (1 heteroatom)]



2*H*-furo[2,3-*d*][1,3]dioxole (PIN)
[dioxole (2 heteroatoms) preferred to furan (1 heteroatom)]

(e) A component containing the greater variety of heteroatoms;

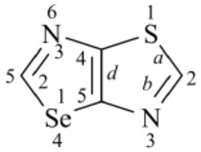
Example:



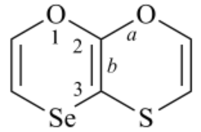
5*H*-[1,3]dioxolo[4,5-*d*][1,2]oxaphosphole (PIN)
[1,3]dioxolo[*d*][1,2]oxaphosphole
(an O and a P atom preferred to two O atoms)

(f) A component containing the greater number of heteroatoms most senior when considered in the order: F > Cl > Br > I > O > S > Se > Te > N > P > As > Sb > Bi > Si > Ge > Sn > Pb > B > Al > Ga > In > Tl.

Examples:



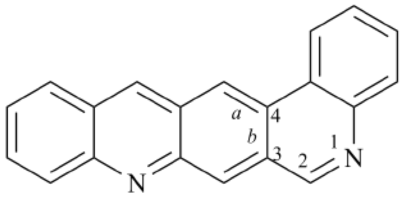
[1,3]selenazolo[5,4-*d*][1,3]thiazole (PIN)
(S,N senior to Se,N)



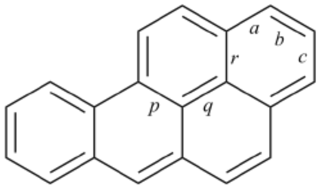
[1,4]oxaselenino[2,3-*b*][1,4]oxathiine (PIN) (O,S senior to O,Se)

(g) A component containing the greatest number of rings in a horizontal row when it is drawn in the preferred orientation according to P-25.3.2.3;

Examples:



quinolino[4,3-*b*]acridine (PIN)
[acridine (3 rings in horizontal row)
preferred to phenanthridine (2 rings in horizontal row)]

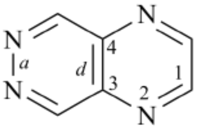


benzo[*pqr*]tetraphene (PIN)

[tetraphene (3 rings in horizontal row)
preferred to chrysene or pyrene (2 rings in horizontal row)]

(h) A component with the lower locants for heteroatoms;

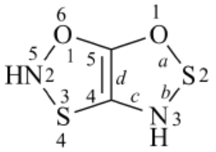
Example:



pyrazino[2,3-*d*]pyridazine (PIN)
(locants ‘1,2’ of pyridazine preferred to locants ‘1,4’ of pyrazine)

(i) A component with the lower locants for the heteroatoms when considered in the order: F > Cl > Br > I > O > S > Se > Te > N > P > As > Sb > Bi > Si > Ge > Sn > Pb > B > Al > Ga > In > Tl;

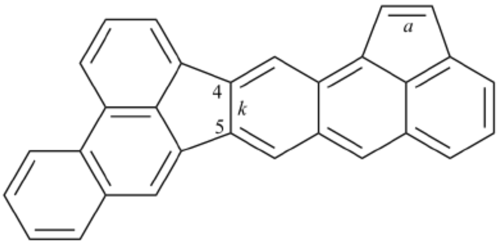
Example:



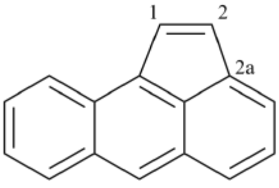
3*H*,5*H*-[1,3,2]oxathiazolo[4,5-*d*][1,2,3]oxathiazole (PIN)
(locants ‘1,2,3’ are lower than ‘1,3,2’)

(j) A component with the lower locants for the peripheral fusion carbon atoms (see P-25.3.3.1 for numbering of fusion carbon atoms).

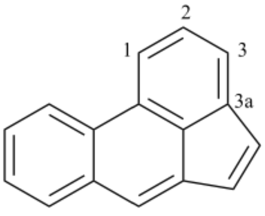
Examples:



acephenanthyleno[5,4-*k*]aceanthrylene (PIN)
(the locant 2a in aceanthrylene is lower than 3a in acephenanthrylene;
see the following structures)



aceanthrylene (PIN)

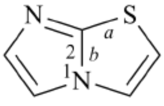


acephenanthrylene (PIN)

P-25.3.2.5 Assembling components and naming fused ring systems. The following criteria are also considered when assembling components and naming fused ring systems.

P-25.3.2.5.1 A heteroatom common to two components must be indicated in the name of each component.

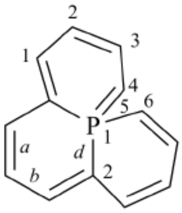
Example:



imidazo[2,1-*b*][1,3]thiazole (PIN)

P-25.3.2.5.2 An atom with a nonstandard bonding number is indicated by the 'λ' (lambda) convention (see P-14.1.3) The nonstandard bonding number *n* is indicated as a superscript to the symbol λ, for example λ^5; this symbol follows the locant of the atom with the nonstandard bonding number in accordance with the numbering of the fused system and is cited at the beginning of the name of the fused ring system.

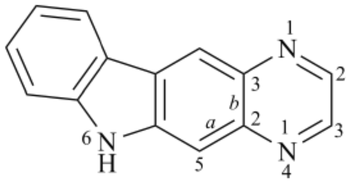
Example:



5λ^5-phosphinino[2,1-*d*]phosphinolizine (PIN)

P-25.3.2.5.3 Indicated hydrogen is cited at the beginning of the name preceded by the appropriate locants of the fused ring system.

Example:



6*H*-pyrazino[2,3-*b*]carbazole (PIN)

P-25.3.3 Numbering fused ring systems

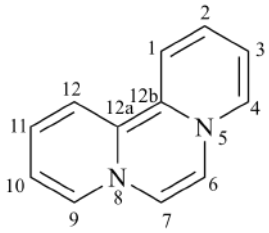
Fused ring systems with retained names, systematic names, or fused names are systematically numbered in the same manner. Anthracene, phenanthrene, acridine, carbazole, xanthene and its chalcogen analogues, purine, and cyclopenta[*a*]phenanthrene are exceptions; traditional numberings are retained. Two types of numbering are to be considered.

P-25.3.3.1 Numbering of peripheral skeletal atoms
P-25.3.3.2 Numbering of interior heteroatoms
P-25.3.3.3 Numbering of interior carbon atoms

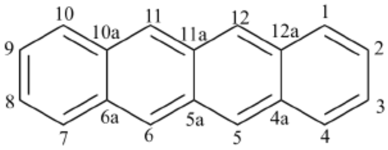
P-25.3.3.1 Numbering of peripheral skeletal atoms

P-25.3.3.1.1 The numbering of peripheral atoms in the preferred orientation starts from the uppermost ring. If there is more than one uppermost ring, the ring furthest to the right is chosen. Numbering starts from the nonfused atom most counterclockwise in the ring selected and proceeds in a clockwise direction around the system, including fusion heteroatoms but not fusion carbon atoms. Each fusion carbon atom is given the same number as the immediately preceding nonfusion skeletal atom, modified by a Roman letter 'a', 'b', 'c', 'd', etc.

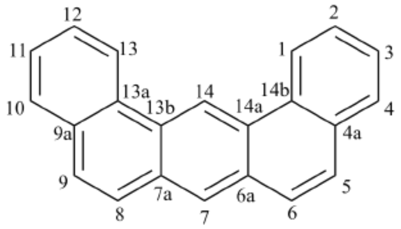
Examples:



dipyrido[1,2-*a*:2′,1′-*c*]pyrazine (PIN)



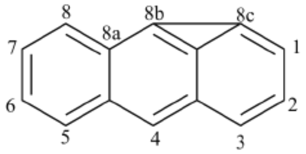
tetracene (PIN)


12
2
11
13
1
3
13a
14
14b
10
13b
14a
4
9a
4a
9
7a
6a
5
8
7
6

benzo[*m*]tetraphene (PIN)

If the uppermost ring does not have a nonfusion atom, then numbering starts in the next ring encountered when proceeding around the system in a clockwise direction.

Example:

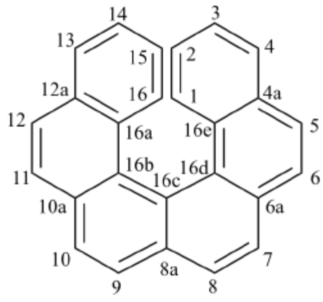

8
8b
8c
8a
7
1
6
2
5
4
3

cyclopropa[*de*]anthracene (PIN)

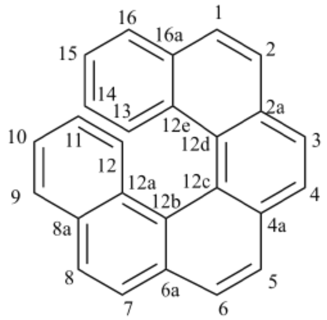
Sections FR-5.3, FR-5.4 and FR-5.5 in ref. 4 describe numbering for more complex structures.

In particular, the orientation and numbering of helicenes has been changed. Recommended numbering and former numbering for hexahelicene are shown below.

Higher helicenes follow the same pattern. A helicene is oriented so that a terminal ring is located in the upper right quadrant; numbering always begins in this terminal ring.


14
3
13
15
2
4
12a
16
1
4a
12
16a
16e
5
16b
16d
11
16c
6
10a
6a
10
8a
7
9
8

hexahelicene (PIN)
(new orientation and numbering)

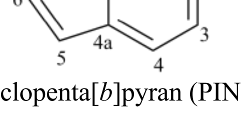

16
1
16a
15
2
14
13
2a
10
11
12e
3
12d
12
12a
12c
9
12b
4
8a
4a
8
6a
5
7
6

Note: Orientation and numbering no longer recommended;
but still in use by CAS for the ring system having the name
phenanthro[3,4-*c*]phenanthrene, ref. 22)

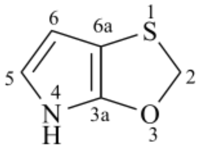
P-25.3.3.1.2 If alternative numberings for a ring system remain after the application of P-25.3.3.1.1 (including alternative locations for heteroatoms), the following criteria are applied in order until a decision is reached:

(a) low locants are assigned to heteroatoms, considered as a set without regard to the kind of heteroatom;

Examples:


1
7
7a
O
2
6
3
5
4a
4

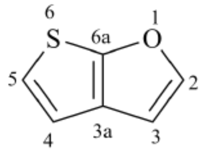
cyclopenta[*b*]pyran (PIN)



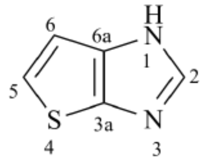
2*H*,4*H*-[1,3]oxathiolo[5,4-*b*]pyrrole (PIN)

(b) low locants are assigned to heteroatoms in the order: F > Cl > Br > I > O > S > Se > Te > N > P > As > Sb > Bi > Si > Ge > Sn > Pb > B > Al > Ga > In > Tl;

Examples:



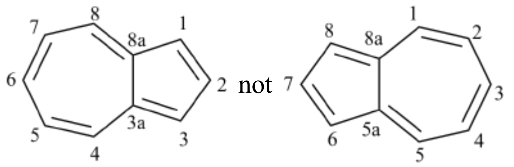
thieno[2,3-*b*]furan (PIN)



1*H*-thieno[2,3-*d*]imidazole (PIN)

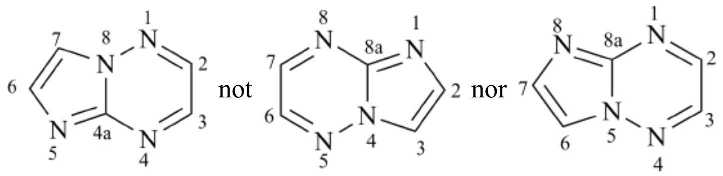
(c) low locants are assigned to fusion carbon atoms;

Examples:



azulene (PIN)

Explanation: The locants '3a,8a' are lower than '5a,8a'.

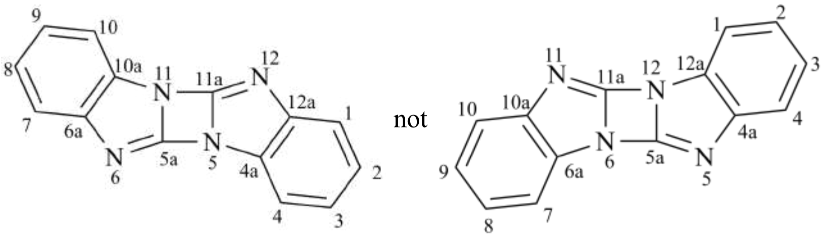


imidazo[1,2-*b*][1,2,4]triazine (PIN)

Explanation: The locant '4a' is lower than '8a'.

(d) low locants are assigned to fusion rather than nonfusion heteroatoms of the same element;

Example:

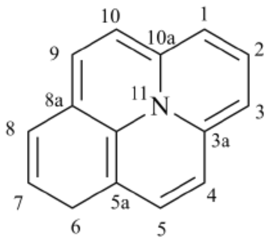


[1,3]diazeto[1,2-*a*:3,4-*a*′]bis([1,3]benzimidazole) (PIN)
[1,3]diazeto[1,2-*a*:3,4-*a*′]dibenzimidazole

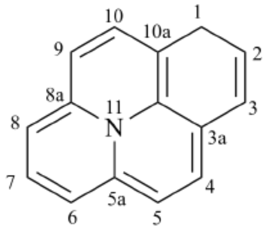
Explanation: The locant '5' is lower than '6'.

(e) low locants are assigned so that an interior heteroatom is nearer (i.e., fewer bonds in the pathway) to the lowest numbered fusion peripheral atom (see P-25.3.3.2 for interior numbering);

Example:


10
1
9
10a
2
8a
11
N
3
8
3a
7
5a
4
6
5

not

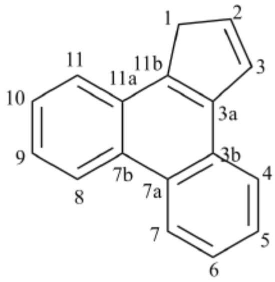

10
1
10a
9
2
8a
11
3
8
N
3a
7
4
5a
6
5

6*H*-quinolizino[3,4,5,6-*ija*]quinoline (PIN)

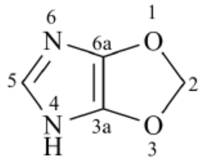
Explanation: The locant ‘3a’ next to the nitrogen atom is lower than ‘5a’.

(f) low locants are assigned to indicated hydrogen atoms (expressed or implied);

Examples:

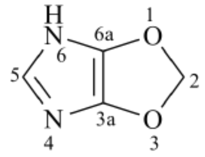

1
2
11
11b
11a
3
10
3a
9
3b
4
7b
8
7a
7
5
6

1*H*-cyclopenta[*l*]phenanthrene (PIN)


6
1
N
6a
O
5
2
4
N
3a
O
H
3

2*H*,4*H*-[1,3]dioxolo[4,5-*d*]imidazole
correct

not


H
1
N
6a
O
6
5
2
N
3a
O
4
3

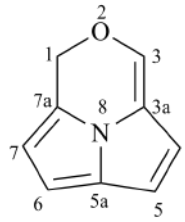
2*H*,6*H*-[1,3]dioxolo[4,5-*d*]imidazole
incorrect

Explanation: The locant set ‘2,4’ for indicated hydrogen atoms is lower than ‘2,6’.

P-25.3.3.2 Numbering of interior heteroatoms

P-25.3.3.2.1 Interior heteroatoms that are not identified by skeletal replacement (‘a’) nomenclature are numbered after the peripheral atoms continuing the established number sequence [see also P-25.3.3.1.2 (e)]. Compare the numbering of interior carbon atoms (see P-25.3.3.3).

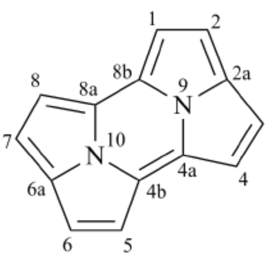
Example:


2
O
1
3
7a
8
3a
N
7
4
6
5a
5

1*H*-[1,4]oxazino[3,4,5-*cd*]pyrrolizine (PIN)

P-25.3.3.2.2 If there is a choice, the shortest pathway in terms of the number of bonds from each heteroatom to the periphery is determined. The lower number is given to the heteroatom whose shortest pathway connects to the lowest numbered peripheral atom.

Example:

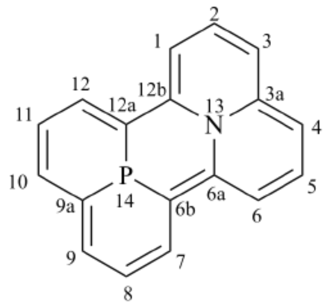

1
2
8b
2a
8
8a
9
N
3
7
N
10
4a
4
6a
4b
6
5

pyrazino[2,1,6-*cd*:3,4,5-*c′d′*]dipyrrolizine (PIN)

Explanation: The heteroatom numbered ‘9’ is one bond away from ‘2a’, which is lower than ‘4b’.

P-25.3.3.2.3 If there is a choice between heteroatoms of different elements, the lower locant is assigned in accordance with the order F > Cl > Br > I > O > S > Se > Te > N > P > As > Sb > Bi > Si > Ge > Sn > Pb > B > Al > Ga > In > Tl;

Example:



1
2
3
12
12b
13
3a
11
12a
N
4
10
P
5
9a
14
6b
6a
6
9
7
8

phosphinolizino[4′,5′,6′:3,4,5][1,4]azaphosphinino[2,1,6-*de*]quinolizine (PIN)

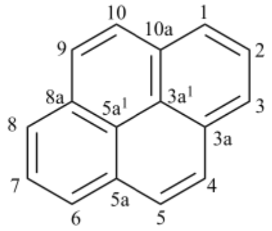
Explanation: The nitrogen atom has a lower locant than the phosphorus atom.

P-25.3.3.3 Numbering of interior carbon atoms

P-25.3.3.3.1 Interior atoms are numbered by identifying the minimum number of bonds linking them to a peripheral atom. The locant for the interior atom is that of the peripheral atom with a superscript number corresponding to the number of bonds between the two atoms. The previous rule (Rule A-22.2 in ref. 1), which is still used in CAS index nomenclature, recommended that interior atoms follow the highest numbered peripheral atom adding Roman letters in sequence to the appropriate peripheral number.

Note: This is a major change to the rules for interior numbering of carbon atoms recommended in the 1998 publication on fusion nomenclature (see FR-5.5.2 in ref. 4).

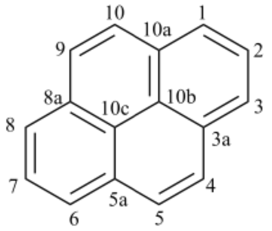
Examples:



10
1
10a
9
2
8a
5a^1
3a^1
3
8
3a
7
5a
4
6
5

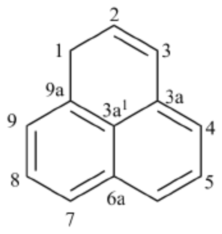
pyrene (PIN)
(recommended numbering)

not



10
1
10a
9
2
8a
10c
10b
3
8
3a
7
5a
4
6
5

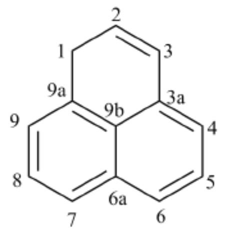
Note: Former numbering, no longer recommended but still used in CAS index nomenclature.



2
1
3
9a
3a
3a^1
9
4
8
5
6a
7

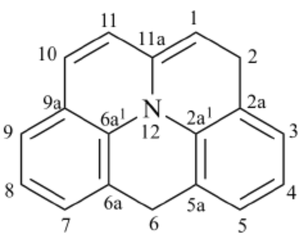
1*H*-phenalene (PIN)
(recommended numbering)

not



2
1
3
9a
3a
9b
9
4
8
5
6a
7
6

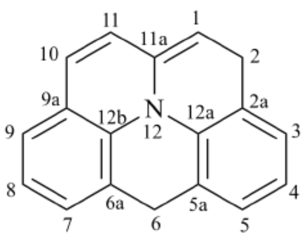
Note: Former numbering, no longer recommended but still used in CAS index nomenclature.



11
1
11a
10
2
9a
N
2a
6a^1
2a^1
9
12
3
8
4
6a
5a
7
6
5

2*H*,6*H*-quinolizino[3,4,5,6,7-*defg*]acridine (PIN)
(recommended numbering)

not

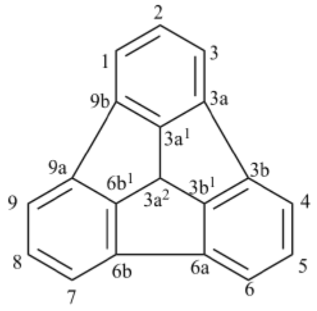


11
1
11a
10
2
9a
12b
N
12a
2a
9
12
3
8
4
6a
5a
7
6
5

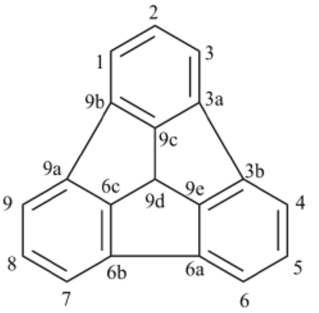
Note: Former numbering, no longer recommended but still used in CAS index nomenclature.

P-25.3.3.3.2 If there is a choice of locants for interior carbon atom, lower locants are selected.

Example:



not



3a^2*H*-benzo[3,4]pentaleno[2,1,6,5-*jklm*]fluorene (PIN)
(recommended numbering)

Note: Former numbering, no longer recommended
but still used in CAS index nomenclature.

P-25.3.4 Constructing polycomponent fusion names

When several nonidentical components must be considered, one, and only one, can be the parent component. All other components are attached components. A component attached directly to the parent component is called a 'first-order attached component'. A component attached to a first-order attached component is called a 'second-order' attached component, and so on. The parent and the first-order attached components are named as indicated for two component systems (see P-25.3.2).

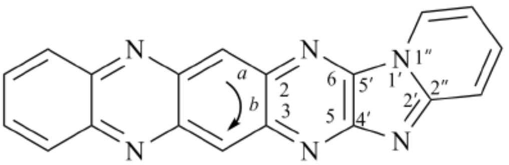
P-25.3.4.1 Three types of fusion names are considered in these recommendations.

P-25.3.4.1.1 Fusion names composed of first- and higher-order attached components
P-25.3.4.1.2 Identical attached components
P-25.3.4.1.3 Multiparent names

P-25.3.4.1.1 Fusion names composed of first- and higher-order attached components

The procedure for indicating common bond(s) between a first-order attached component and a higher-order attached component follows that for the attachment of the parent compound to the first-order attached component except that numerical locants are used instead of letters and the two sets of locants are separated by a colon. The locants of second-order attached components are primed to contrast with those of first-order attached components. The locants of third-order attached components are doubly primed, and so on.

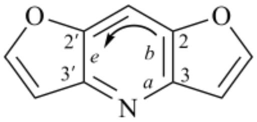
Example:



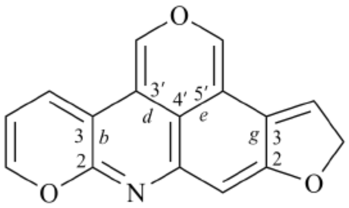
pyrido[1″,2″:1′,2′]imidazo[4′,5′:5,6]pyrazino[2,3-*b*]phenazine (PIN)

P-25.3.4.1.2 Identical attached components
A multiplicity of components that are identical and are all fused to a parent component or an attached component is indicated by the use of the prefix 'di', 'tri', etc. (or 'bis', 'tris', etc.). The multiplying prefix is not considered in determining the alphabetical order of attached components in names of polycomponent fusion names (see P-25.3.4.2.3). A colon separates the sets of locants, and a comma is used when letters only are present.

Examples:



difuro[3,2-*b*:2′,3′-*e*]pyridine (PIN)



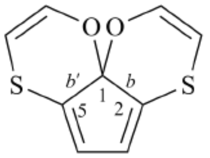
5*H*-furo[3,2-*g*]dipyrano[2,3-*b*:3′,4′,5′-*de*]quinoline (PIN)
(furo before dipyrano)

P-25.3.4.1.3 Multiparent names

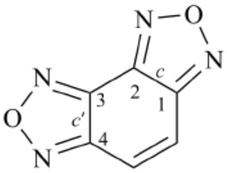
Multiple occurrences of the parent component in a multiparent system is indicated by the use of multiplying prefixes, ‘di’, ‘tri’, etc, or ‘bis’, ‘tris’, etc. To distinguish between the parent components, the second has primed locants, the third double primed, etc.

The use of enclosing parentheses following ‘di’, ‘tri’, etc., indicating multiple occurrences of a parent component in these recommendations is a change from the recommendations in the 1998 publication on fusion nomenclature (ref. 4).

Examples:



cyclopenta[1,2-*b*:1,5-*b*′]bis([1,4]oxathiine) (PIN)



benzo[1,2-*c*:3,4-*c*′]bis([1,2,5]oxadiazole) (PIN)

P-25.3.4.2 Constructing polycomponent fusion names

Polycomponent fusion names are constructed by using specific orders of seniority and rules. They are elaborated as follows.

P-25.3.4.2.1 Order of seniority for selecting parent components
P-25.3.4.2.2 Order of seniority for selecting attached components
P-25.3.4.2.3 Order of citation of fusion prefixes
P-25.3.4.2.4 Order of seniority of locants (letters and numbers)

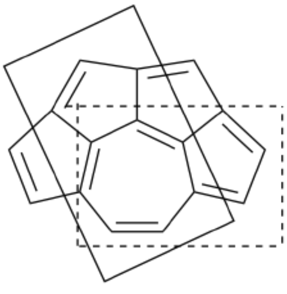
P-25.3.4.2.1 Order of seniority for selecting parent components

When there are two or more locations for a parent component in a fused ring structure, the following criteria are applied sequentially until a complete distinction is obtained. In the examples below, the senior location is identified by a solid box and other locations with a dashed box.

The senior location is:

(a) the location that enables the whole ring system to be named by fusion nomenclature, thus excluding names of bridged fused systems;

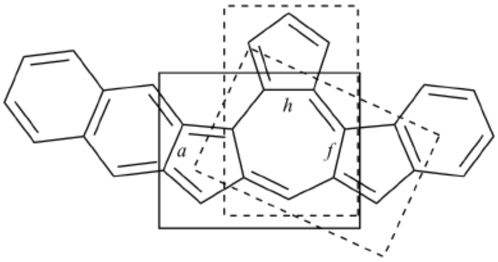
Example:



cyclopenta[*ij*]pentaleno[2,1,6-*cde*]azulene (PIN)
(not 1,9-methenopentaleno[1,6-*ef*]azulene
nor 1,9-methenodicyclopenta[*cd*,*f*]azulene;
names including the prefix ‘metheno’ are bridged fused ring names)

(b) the location that results in a name that does not require attached components higher than first-order. For didactic purposes only, names of attached components of higher order than first-order are written in bold type;

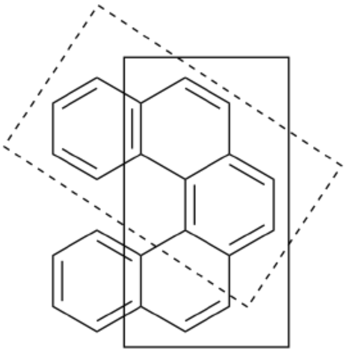
Example:



cyclopenta[*h*]indeno[2,1-*f*]naphtho[2,3-*a*]azulene (PIN)
(not benzo[*a*]**benzo**[5,6]indeno[2,1-*f*]cyclopenta[*h*]azulene
nor **benzo**[5,6]indeno[1,2-*e*]indeno[2,1-*h*]azulene;
there is no second-order component in the recommended name)

(c) the location that results in the maximum number of first-order attached components, second-order attached components, etc. This criterion results in the minimum number of higher-order attached components; hence, fewer primed fusion descriptors are required;

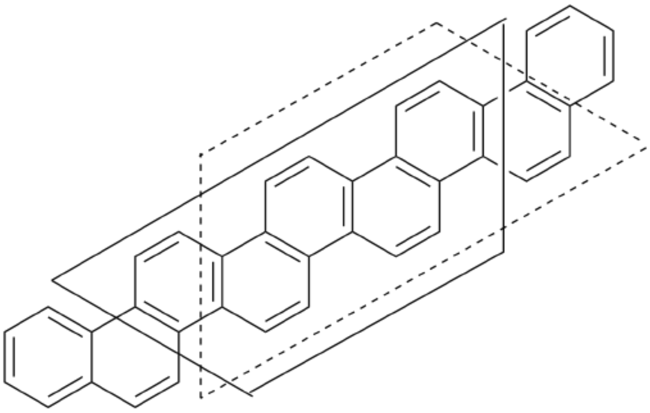
Example:



dibenzo[*c*,*g*]phenanthrene
(not naphtho[2,1-*c*]phenanthrene;
two attached components preferred to one)

(d) a location that permits the expression of the maximum number of identical attached components with multiplicative prefixes;

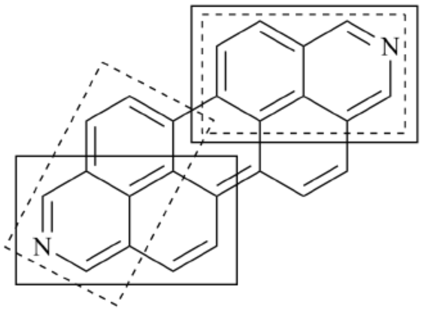
Example:



dinaphtho[1,2-*c* :2′,1′-*m*]picene (PIN)
(not benzo[*c*]phenanthreno[2,1-*m*]picene)

(e) a location that uses a senior interparent component;

Example:



anthra[2,1,9-*def*:6,5,10-*d′e′f′*]diisoquinoline (PIN)
(not phenanthro[2,1,10-*def*:7,8,9-*d′e′f′*]diisoquinoline;
anthracene is senior to phenanthrene)

(f) a location that results in preferred attached components, first-order, then second-order, etc. This criterion is embellished and illustrated in the original publication (see FR-3.3.1 in ref. 4).

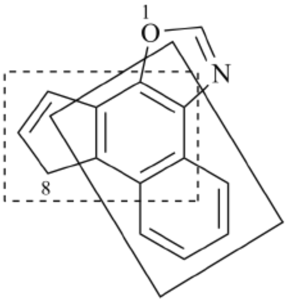
P-25.3.4.2.2 Order of seniority for selecting attached components

After selection of the parent component (see P-25.3.2.4) [or parent components and interparent component(s) if a multiparent name is chosen], other rings are identified as far as possible as attached components. If there is a choice, first-order attached components are considered first, then second-order attached components, etc. The following criteria are applied in order only until a complete decision is made:

Note: In the examples below, the preferred attached component is marked with a solid box and the alternatives with dashed boxes.

(a) if there are alternative first-order attached components, the senior ring or ring system is selected. The same procedure is applied to second-order attached components, and so on;

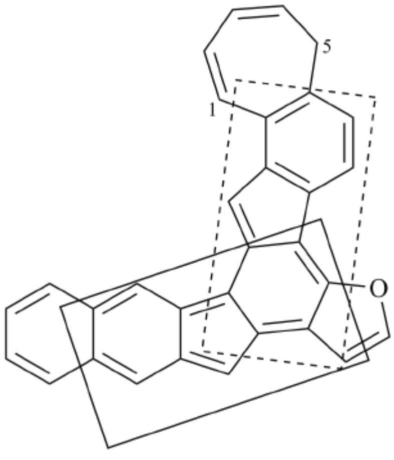
Example:



8*H*-cyclopenta[3,4]naphtho[1,2-*d*][1,3]oxazole (PIN)
(not 8*H*-benzo[6,7]indeno[5,4-*d*][1,3]oxazole;
naphthalene is senior to indene)

(b) the location that has lowest locants as a set for fusion of first-order attached components to the parent component;

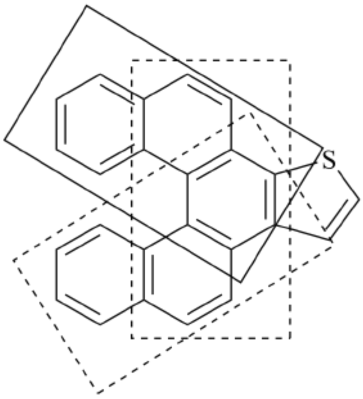
Example:



5*H*-benzo[6,7]cyclohepta[4′,5′]indeno[1′,2′:3,4]fluoreno[2,1-*b*]furan (PIN)
(not 5*H*-benzo[5′,6′]indeno[1′,2′:1,2]cyclohepta[7,8]fluoreno[4,3-*b*]furan;
locants 1,2 are lower than 3,4 for the ‘fluoreno’ attached component)

(c) the location that has lowest locants for fusion to the parent component in order of citation.

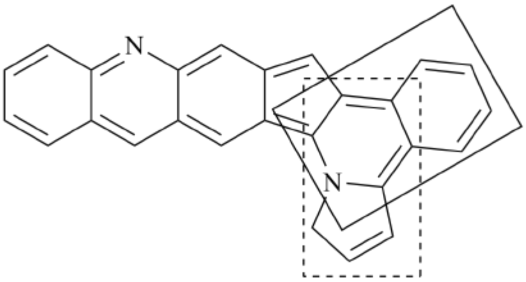
Example:



naphtho[2′,1′:3,4]phenanthro[1,2-*b*]thiophene (PIN)
(not naphtho[2′,1′:3,4]phenanthro[2,1-*b*]thiophene,
not dibenzo[3,4:5,6]phenanthro[9,10-*b*]thiophene;
the locants ‘1,2’ for the ‘phenanthro’ attached component, in order of citation, are lower than ‘2,1’ or ‘9,10’)

This procedure is continued exploring outwards to the senior second-order attached components.

Example:

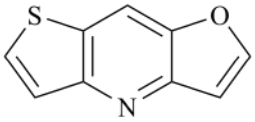


7*H*-pyrrolo[2″,1″:1′,2′]isoquinolino[4′,3′:4,5]cyclopenta[1,2-*b*]acridine (PIN)
(not 7*H*-benzo[7′,8′]indolizino[6′,5′:4,5]cyclopenta[1,2-*b*]acridine;
isoquinoline is senior to indolizine)

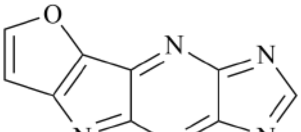
P-25.3.4.2.3 Order of citation of fusion prefixes

P-25.3.4.2.3.1 Fusion between two attached components is indicated by the method described in P-25.3.2. All attached components are cited in front of the parent component. Each second-order attached component is cited in front of the first-order attached component to which it is fused, and so on to higher order attached components. If there are two or more different components, or sets of components, attached to a lower order component, they are cited in alphabetical order.

Examples:

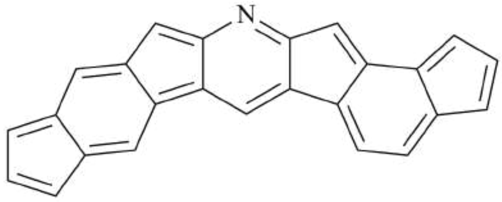


furo[3,2-*b*]thieno[2,3-*e*]pyridine (PIN)
(furo is cited before thieno)



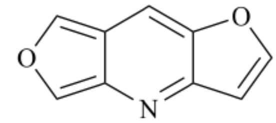
furo[2′,3′:4,5]pyrrolo[2,3-*b*]imidazo[4,5-*e*]pyrazine (PIN)
(furo...pyrrolo is cited before imidazo)

Note: In the case of the indacenes, if the only distinction is between *as*-indacene and *s*-indacene, then the italic characters are considered. Otherwise, they are treated as indacene for consideration of alphabetical order. It should be noted that *s*-indacene is senior to *as*-indacene in the order of seniority of components.

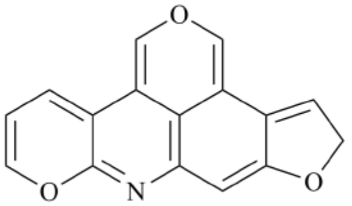


as-indaceno[2,3-*b*]-*s*-indaceno[1,2-*e*]pyridine (PIN)

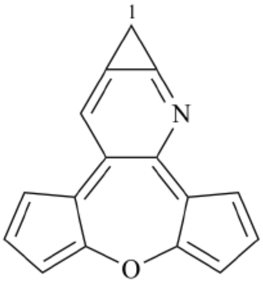
P-25.3.4.2.3.2 If two or more identical components are fused to a third component, they are cited together using multiplying prefixes (‘di’, ‘tri’, etc.; or ‘bis’, ‘tris’, etc.). The citation of different components is in alphabetical order of the names of the components, just as for simple multiplicative prefixes in substitutive nomenclature. The multiplicative prefix is considered only when it is an integral part of a multipart fusion prefix.



difuro[3,2-*b*:3′,4′-*e*]pyridine (PIN)



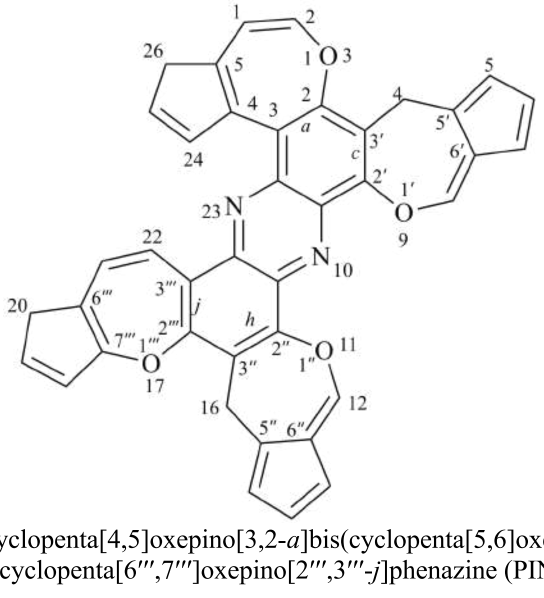
5*H*-furo[3,2-*g*]dipyrano[2,3-*b*:3′,4′,5′-*de*]quinoline (PIN)
(furo is cited before pyrano)



1*H*-cyclopropa[*b*]dicyclopenta[2,3:6,7]oxepino[4,5-*e*]pyridine (PIN)
(not 1*H*-dicyclopenta[2,3:6,7]oxepino[4,5-*b*]cyclopropa[*e*]pyridine;
cyclopropa is cited before dicyclopentaoxepino, which is treated as one component)

P-25.3.4.2.3.3 If two or more groups of components differ only by virtue of the fusion locants within the group, these locants are used to determine the order of citation of prefixes; lower locant sets are cited earlier.

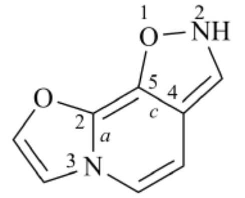
Example:



4*H*,16*H*,20*H*,26*H*-cyclopenta[4,5]oxepino[3,2-*a*]bis(cyclopenta[5,6]oxepino)[3′,2′-*c*:2″,3″-*h*]cyclopenta[6‴,7‴]oxepino[2‴,3‴-*j*]phenazine (PIN)

P-25.3.4.2.3.4 If two or more groups of components only differ by virtue of heteroatom locants, these locants are used to determine the order; lower locant sets are cited earlier.

Example:



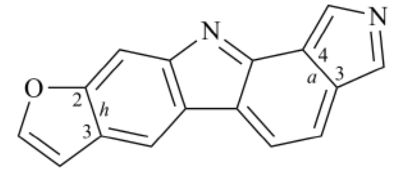
2*H*-[1,2]oxazolo[5,4-*c*][1,3]oxazolo[3,2-*a*]pyridine (PIN)

P-25.3.4.2.4 Order of seniority of locants (letters and numbers)

If there is a choice of locants, letters, or numerals (consistent with the numbering of the component), the lower letters or numbers are selected in accordance with the following criteria, which are considered in order until a complete decision can be made:

(a) parent component letters as a set;

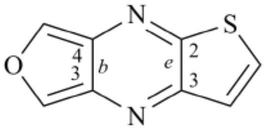
Example:



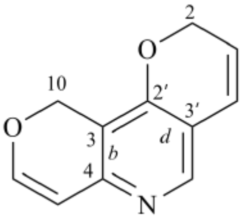
furo[3,2-*h*]pyrrolo[3,4-*a*]carbazole (PIN)
(not furo[2,3-*b*]pyrrolo[3,4-*i*]carbazole;
a,*h* is lower than *b*,*i*)

(b) Parent component letters in order of citation;

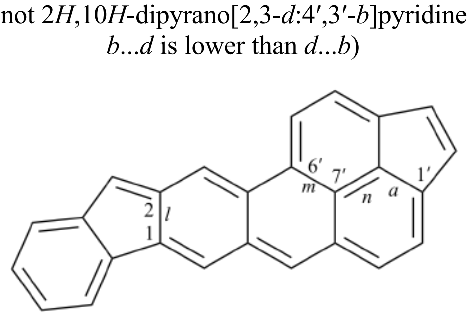
Examples:



furo[3,4-*b*]thieno[2,3-*e*]pyrazine (PIN)
(not furo[3,4-*e*]thieno[2,3-*b*]pyrazine;
b...*e* is lower than *e*...*b*)



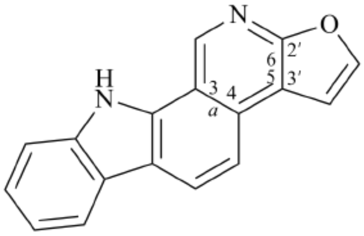
2*H*,10*H*-dipyrano[4,3-*b*:2′,3′-*d*]pyridine (PIN)
(not 2*H*,10*H*-dipyrano[2,3-*d*:4′,3′-*b*]pyridine;
b...*d* is lower than *d*...*b*)



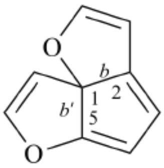
diindeno[1,2-*i*:6′.7′,1′-*mna*]anthracene (PIN)
(not diindeno[6,7,1-*mna*:1′,2′-*i*]anthracene;
i...*mna* is lower than *mna*...*i*)

(c) Set of locants of the first-order attached components for fusion to the parent component;

Examples:



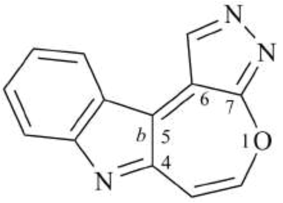
10*H*-furo[3′,2′:5,6]pyrido[3,4-*a*]carbazole (PIN)
(not 10*H*-furo[2′,3′:2,3]pyrido[5,4-*a*]carbazole;
the locant set ‘3,4’ is lower than ‘4,5’ for attaching pyrido to carbazole)



cyclopenta[1,2-*b*:5,1-*b*′]difuran (PIN, a multiparent name)
(not cyclopenta[1,2-*b*:2,3-*b*′]difuran;
the locant set ‘1,1,2,5’ is lower than ‘1,2,2,3’)

(d) First-order attached component locants for fusion to the parent component in order of citation;

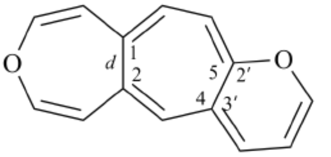
Example:



pyrazolo[4′,3′:6,7]oxepino[4,5-*b*]indole (PIN)
(not pyrazolo[3′,4′:2,3]oxepino[5,4-*b*]indole;
the locant set ‘4,5’ is lower than ‘5,4’)

(e) Locants for lower-order attached components as a set for fusion to higher-order attached component;

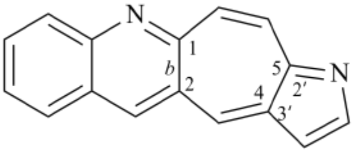
Example:



pyrano[3′,2′:4,5]cyclohepta[1,2-*d*]oxepine (PIN)
(not pyrano[2′,3′:5,6]cyclohepta[1,2-*d*]oxepine;
the locant set ‘4,5’ is lower than ‘5,6’)

(f) Locants for lower-order attached components for fusion to higher-order attached components in order of citation;

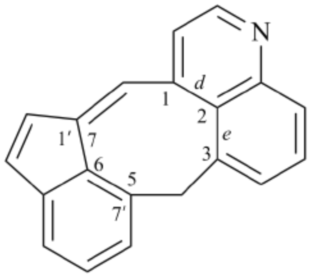
Example:



pyrrolo[3′,2′:4,5]cyclohepta[1,2-*b*]quinoline (PIN)
(not pyrrolo[2′,3′:5,4]cyclohepta[1,2-*b*]quinoline;
the locant set ‘4,5’ is lower than ‘5,4’)

(g) Locants for higher-order attached components as a set for fusion to the lower-order attached component.

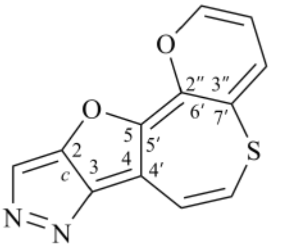
Example:



7*H*-indeno[7′,1′:5,6,7]cycloocta[1,2,3-*de*]quinoline (PIN)
(not 7*H*-indeno[3′,4′:5,6,7]cycloocta[1,2,3-*de*]quinoline;
the locant set ‘1′,7′’ is lower than ‘3′,4′’)

(h) Locants for higher-order components in fusion to lower-order components in order of citation.

Example:



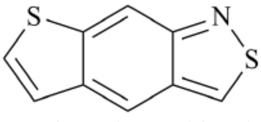
pyrano[2″,3″:6′,7′]thiepino[4′,5′:4,5]furo[3,2-*c*]pyrazole (PIN)
(not pyrano[3″,2″:2′,3′]thiepino[5′,4′:4,5]furo[3,2-*c*]pyrazole;
the locant set ‘4′,5′’ is lower than ‘5′,4′’)

P-25.3.5 Heteromonocyclic rings fused to a benzene ring

Heterobicyclic compounds consisting of a heteromonocycle fused to a benzene ring in which the benzene ring is not part of a system having a retained name such as quinoline or naphthalene are treated as a single component unit (a ‘benzoheterocycle’, see P-25.2.2.4). They may be treated as a parent component or an attached component depending on the order of seniority described in P-25.3.2.4. However, this approach is not used if it disrupts a multiparent system (see P-25.3.5.3, below) or the use of multiplicative prefixes (see P-25.3.6.1, below).

P-25.3.5.1 A benzoheterocycle as a parent component

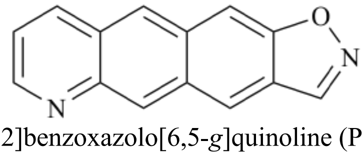
Example:



thieno[3,2-*f*][2,1]benzothiazole (PIN)
(2,1-benzothiazole is senior to 1-benzothiophene)

P-25.3.5.2 A more senior component as parent component

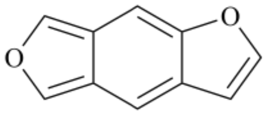
Example:



[1,2]benzoxazolo[6,5-*g*]quinoline (PIN)
(quinoline is senior to 1,2-benzoxazole)

P-25.3.5.3 A multiparent name is preferred to a fused ring system, when there is a choice.

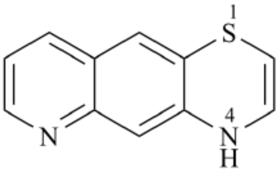
Example:



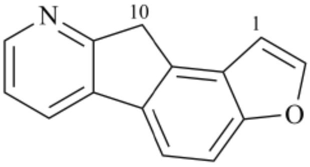
benzo[1,2-*b*:4,5-*c*′]difuran (PIN)
(not furo[3,4-*f*][1]benzofuran;
a multiparent name is preferred to a two-component fused name)

P-25.3.5.4 Retained names are senior to names of benzoheterocycles.

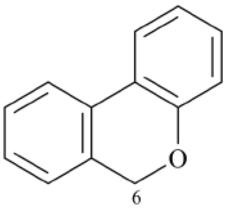
Examples:



4*H*-[1,4]thiazino[2,3-*g*]quinoline (PIN)
(the retained name quinoline must be used)



10*H*-furo[3′,2′:4,5]indeno[2,1-*b*]pyridine (PIN)
(not 10*H*-[1]benzofuro[5′,4′:3,4]cyclopenta[1,2-*b*]pyridine;
pyridine is senior to furan; indene, as a retained name, must be used)

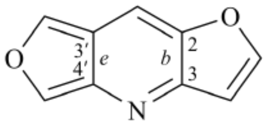


6*H*-dibenzo[*b*,*d*]pyran (PIN)
(not 6*H*-benzo[*c*][1]benzopyran;
not 6*H*-benzo[*c*][2]benzopyran)
6*H*-benzo[*c*]chromene

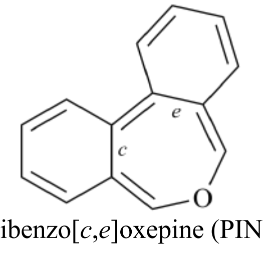
P-25.3.6 Identical attached components

P-25.3.6.1 Two or more components that are identical and both fused to a parent component are indicated by the use of multiplying prefixes (‘di’, ‘tri’, etc. or ‘bis’, ‘tris’, etc.). If a complete set of locants is used for first-order attached components fused to the parent component, they are cited together separated by a colon. If abbreviated sets of locants are used, the letters are separated by a comma. If complete sets of locants are used for second-order attached components fused to a first-order attached component, or for higher-order cases, the locants are cited together separated by a semicolon. If abbreviated sets are used, they are separated by a colon. To distinguish between two or more components of the same order, the locants of the second component are primed (or double primed if the first is primed, etc.), the third double primed, and so on.

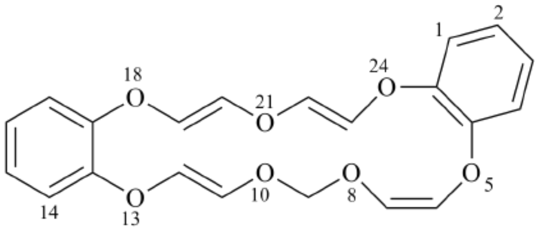
Examples:



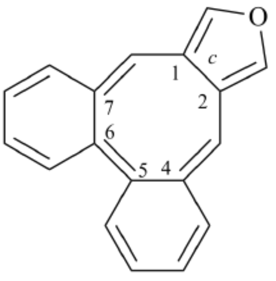
difuro[3,2-*b*:3′,4′-*e*]pyridine (PIN)



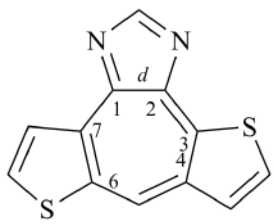
dibenzo[*c*,*e*]oxepine (PIN)


1
2
18
24
21
O
O
O
O
O
O
O
5
10
8
14
13

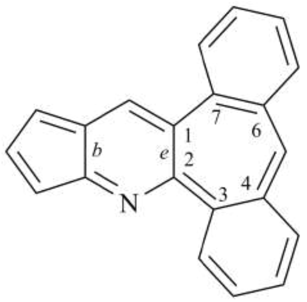
9*H*-dibenzo[*g*,*p*][1,3,6,9,12,15,18]heptaoxacycloicosine (PIN)



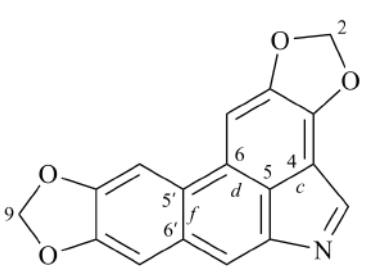
dibenzo[4,5:6,7]cycloocta[1,2-*c*]furan (PIN)


N
N
d
1
2
7
S
3
4
6
S

dithieno[2′,3′:3,4;2″,3″:6,7]cyclohepta[1,2-*d*]imidazole (PIN)



cyclopenta[*b*]dibenzo[3,4:6,7]cyclohepta[1,2-*e*]pyridine (PIN)

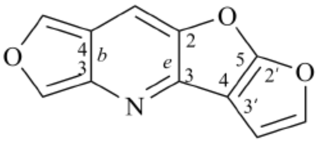

O
2
O
6
5
4
O
5′
d
c
9
f
6′
O
N

2*H*,9*H*-bis([1,3]benzodioxolo)[4,5,6-*cd*:5′,6′-*f*]indole (PIN)

P-25.3.6.2 Additional components attached to a system with a multiplicative prefix.

Fusion of a higher-order attached component to a system named with a multiplicative prefix requires each set of attached components to be specified separately.

Example:

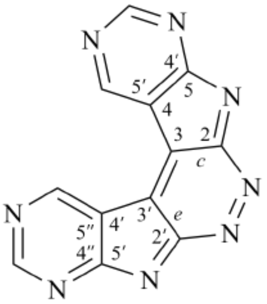

O
4
3
b
e
2
3
O
5
2′
O
4
3′
N

furo[3,4-*b*]furo[3′,2′:4,5]furo[2,3-*e*]pyridine (PIN)

P-25.3.6.3 Identical components with identical fusion locants.

Two or more groups of identical components (including identical fusion locants between these components) fused to another component, are indicated by the use of the multiplying prefixes ‘bis’, ‘tris’, etc., and the group of components is cited within parentheses.

Example:



bis(pyrimido[5′,4′:4,5]pyrrolo)[2,3-*c*:3′,2′-*e*]pyridazine (PIN)

P-25.3.7 Multiparent ring systems

Multiple occurrences of the parent component in a multiparent system is indicated by the use of multiplying prefixes, ‘di’, ‘tri’, etc., or ‘bis’, ‘tris’, etc. To distinguish between the parent components, the second has primed locants, the third double primed, etc.

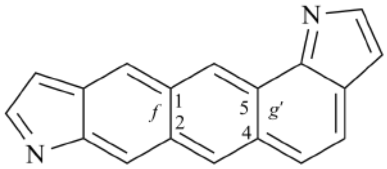
Two or more nonoverlapping locations for parent components that are *ortho*- or *ortho*- and *peri*-fused to the same first-order interparent component are treated as a multiparent system and given a multiparent name. Similarly a system with three, five, seven, etc. interparent components is treated as an extended multiparent system. Each pair of second- or higher-order interparent components must be identical.

P-25.3.7.1 Multiparent systems with one interparent component

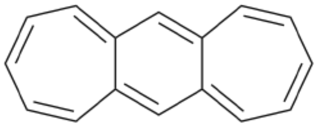
Multiple occurrences of the parent component in a multiparent system are indicated by the use of a multiplying prefix (‘di’, ‘tri’, etc., or ‘bis’, ‘tris’, etc.). To distinguish between the parent components, the second parent component has primed letters, the third double primed, etc.; the sets of locants are separated by a colon.

The use of enclosing parentheses following ‘bis’, ‘tris’, etc. indicating multiple occurrences of a parent component in these recommendations is a change from the recommendations in the 1998 publication on fusion nomenclature (ref. 4).

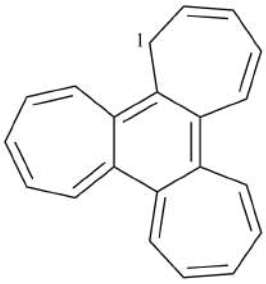
Examples:



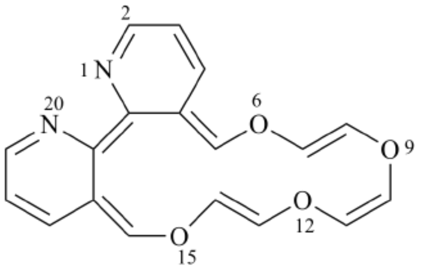
benzo[1,2-*f*:4,5-*g*′]diindole (PIN)



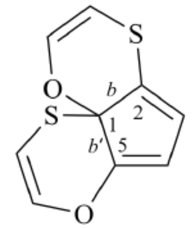
benzo[1,2:4,5]di[7]annulene (PIN)



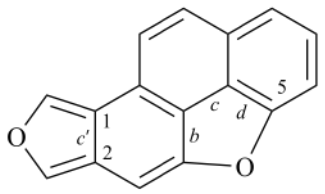
1*H*-benzo[1,2:3,4:5,6]tri[7]annulene (PIN)



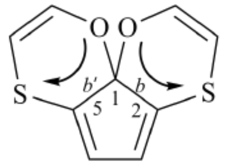
[1,4,7,10]tetraoxacyclohexadecino[13,12-*b*:14,15-*b*′]dipyridine (PIN)



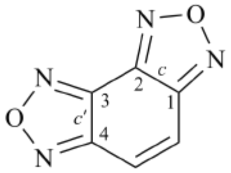
cyclopenta[1,2-*b*:5,1-*b*′]bis([1,4]oxathiine) (PIN)



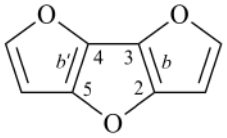
phenanthro[4,5-*bcd*:1,2-*c*′]difuran (PIN)



cyclopenta[1,2-*b*:1,5-*b*′]bis([1,4]oxathiine) (PIN)



benzo[1,2-*c*:3,4-*c*′]bis([1,2,5]oxadiazole) (PIN)

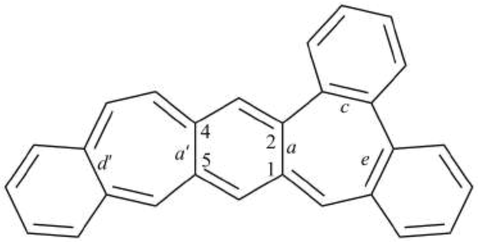


furo[3,2-*b*:4,5-*b*′]difuran (PIN, a multiparent name)
[not difuro[3,2-*b*:2′,3′-*d*]furan (a multiplicative prefix name);
the multiparent method applies to situations in which there are three identical fused rings
or ring systems according to the principle that a maximum of parent components is preferred
to a maximum of attached components]

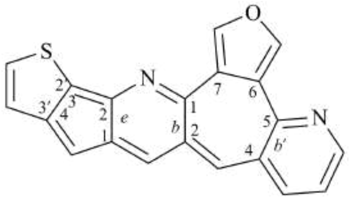
P-25.3.7.2 Additional attached components

Additional attached components may be fused to any of the components of a multiparent system. If the choice of locants described in P-25.3.4.2.4 does not permit a final choice, seniority is given to the unprimed component and the fusion letters are assigned with the lower letter used for fusion to the connecting component. Great care is needed with the use of primes, double primes, etc. to ensure that there is no ambiguity. Thus additional components fused to the interparent component(s) are cited in front of the prefix for the interparent component.

Examples:



tribenzo[*c*,*d*′,*e*]benzo[1,2-*a*:4,5-*a*′]di[7]annulene (PIN)



thieno[2′,3′:3,4]cyclopenta[1,2-*e*]furo[3′,4′:6,7]cyclohepta[1,2-*b*:5,4-*b*′]dipyridine (PIN)
(the furan ring is fused to the interparent component; thus, alphabetical order does not apply)

P-25.3.7.3 Multiparent ring systems with three or more interparent components

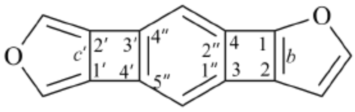
When two (or more) possible parent components are separated by an odd number of interparent components and these are ordered symmetrically with respect to their component rings (but not necessarily with their fusion locants), the whole system is treated as a multiparent system. Names are formed by extending P-25.3.7.1 in two ways as follows:

(a) Second- and higher-order interparent components are named using the multiplying prefixes ‘di’, ‘tri’, etc., or ‘bis’, ‘tris’, etc. Appropriate locants are assigned to interparent components, unprimed and primed for first-order interparent components, double primed for second-order interparent components, tripled primed for third-order interparent components, and so on.

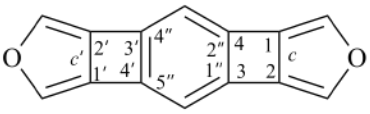
(b) When symmetry permits grouping of interparent components and parent components, such groups can be formed and cited as such using the multiplying prefixes ‘bis’, ‘tris’, etc. to denote groups that are enclosed within parentheses. Unprimed locants only are used within such groupings.

For the method used in generating preferred IUPAC names, see P-52.2.4.3.

Examples:



benzo[1″,2″:3,4;4″,5″:3′,4′]dicyclobuta[1,2-*b*:1′,2′-*c*′]difuran (PIN)

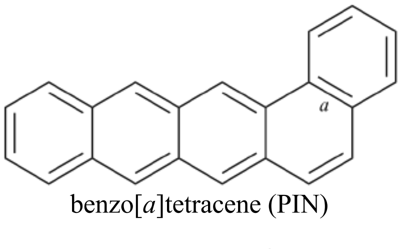


benzo[1″,2″:3,4;4″,5″:3′,4′]bis(cyclobuta[1,2-*c*]furan)

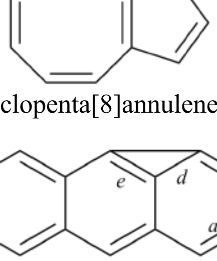
P-25.3.8 Omission of locants in fusion descriptors

P-25.3.8.1 In preferred IUPAC names and in general nomenclature, numerical and/or letter locants are omitted in fused ring systems with only first-order monocyclic attached hydrocarbon components, ‘benzo’, and those described in P-25.3.2.2.1; the omission is also recommended when the fused ring system is made of two monocyclic hydrocarbons.

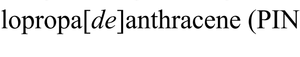
Examples:



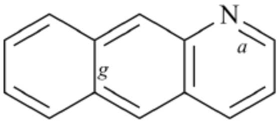
benzo[*a*]tetracene (PIN)



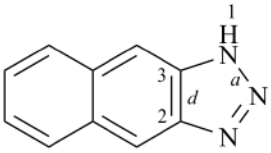
1*H*-cyclopenta[8]annulene (PIN)



cyclopropa[*de*]anthracene (PIN)



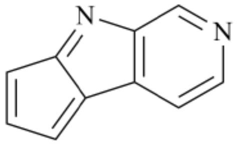
benzo[*g*]quinoline (PIN)



1*H*-naphtho[2,3-*d*][1,2,3]triazole (PIN)
(not 1*H*-naphtho[2,3][1,2,3]triazole)

P-25.3.8.2 Locants are also omitted for the fusion of a terminal monocyclic attached hydrocarbon component.

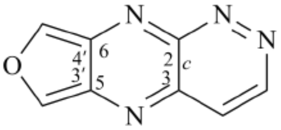
Example:



cyclopenta[4,5]pyrrolo[2,3-*c*]pyridine (PIN)

P-25.3.8.3 When locants are required for the fusion of a second-order or higher-order component then all locants for linking components must be cited.

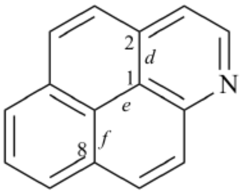
Example:



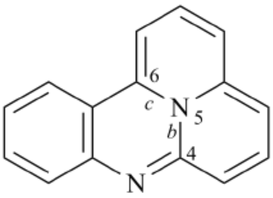
furo[3′,4′:5,6]pyrazino[2,3-*c*]pyridazine (PIN)

P-25.3.8.4 The numerical locants of peripheral fusion carbon atoms of a component are omitted with an *ortho*- and *ortho*- and *peri*-fused system.

Examples:



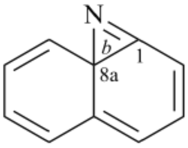
naphtho[2,1,8-*def*]quinoline (PIN)



quinolizino[4,5,6-*bc*]quinazoline (PIN)

Both terminal fusion atom locants for ortho-fusion must be cited even if one is a fusion atom.

Example:



naphtho[1,8a-*b*]azirine (PIN)

P-25.4 BRIDGED FUSED RING SYSTEMS

This Section is based on the publication ‘Nomenclature of Fused and Bridged Fused Ring Systems’ (ref. 4). Sections P-25.4.2.1.2, P-25.4.2.1.4 and P-25.4.2.2.1 contain modifications to Section FR-8.3 of the 1998 publication (ref. 4). No other modifications have been made to the 1998 publication.

P-25.4.1 Definitions and terminology
P-25.4.2 Names of bridges
P-25.4.3 Naming bridged fused ring systems
P-25.4.4 Numbering bridge atoms
P-25.4.5 Order for numbering of bridges

P-25.4.1 Definitions and terminology

P-25.4.1.1 Bridged fused ring system. A ring system in which some of the rings constitute a fused ring system (see P-25.0 through P-25.3) and the remaining rings are created by one or more bridges.

P-25.4.1.2 Bridge. An atom or group of atoms is named as a bridge by means of a prefix if it fulfills one or more of the following:

(a) if it connects two or more nonadjacent positions of the same ring in a fused ring system;

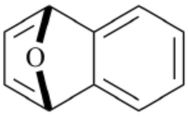
(b) if it connects two or more positions of different rings of a fused ring system and does not thereby form a new *ortho*- and *peri*-fused ring;

(c) if it connects positions of a ring of a fused ring system to a previously described bridge but cannot be included as part of that bridge;

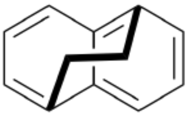
(d) if it connects the atoms at the end of a bond common to two rings of a fused ring system;

(e) if it is used to describe a system with only *ortho*- or *ortho*- and *peri*- fusions that cannot be named entirely by fusion principles.

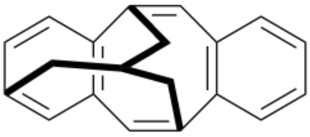
Examples (bridges are indicated in bold):



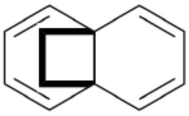
criterion (a)



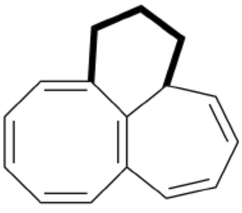
criterion (b)



criterion (c)



criterion (d)



criterion (e)

P-25.4.1.3 Bridgehead atom. An atom of a fused ring system to which a bridge is attached.

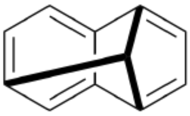
P-25.4.1.4 Simple bridge A bridge that describes an atom, or groups of atoms, which may be described as a single unit, for example ‘epoxy’, ‘butano’, ‘benzeno’.

P-25.4.1.5 Composite bridge. A group of atoms that can only be described as a contiguous sequence of simple bridges, for example (epoxymethano) = epoxy + methano = –O-CH$_2$–.

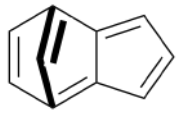
P-25.4.1.6 Divalent bridge. A bridge that is connected by single bonds to two different positions of a fused ring system or bridged fused ring system. All bridges described in P-25.4.2.1 are simple bridges.

P-25.4.1.7 Polyvalent bridge. A bridge that is connected to a fused ring system by three or more single bonds or their multiple bond equivalent. Polyvalent bridges may often be described by a combination of two simple divalent bridges. Polyvalent bridges may be further classified as bipodal, tripodal, etc., when the bridge is attached to two, three, or more positions of the fused ring system.

Examples:



a tripodal trivalent bridge

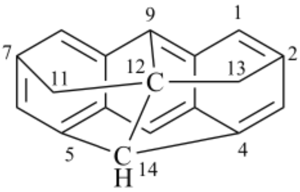


a bipodal trivalent bridge

P-25.4.1.8 Independent bridge. A bridge that only connects two or more positions of a fused ring system (see dependent bridge).

P-25.4.1.9 Dependent bridge. A bridge that connects one or more positions of a fused ring system to one or more positions of a simple or composite independent bridge, and cannot be expressed as part of a larger composite bridge.

Example:



4,5,12-epimethanetriyl-2,9,7-epipropane[1,2,3]triylanthracene (PIN)
(the epimethanetriyl bridge C-14 is a dependent bridge;
the epipropane[1,2,3]triyl bridge at C-11 to C-13 is an independent bridge;
see P-25.4.3.2 for attachment locants)

P-25.4.2 Names of bridges

The extensive list of bridge names given in the publication on fused ring and bridged fused ring nomenclature (ref. 4) has been thoroughly reviewed and updated in the context of the recommendations given herein. Most of the changes occur in the names of acyclic heteroatom bridge names, for which see P-25.4.2.1.4 and P-25.4.2.2.1. For the use of skeletal replacement (‘a’) nomenclature for naming bridges, see P-25.5.1.2.

P-25.4.2.1 Divalent bridges.

P-25.4.2.1.1 A divalent acyclic hydrocarbon bridge is named as a prefix derived from the corresponding unbranched hydrocarbon name by changing the final letter ‘e’ to ‘o’. The locant for a double bond, if present, is indicated in square brackets between the hydrocarbon prefix and the ending ‘eno’; this locant is not the locant used in the final numbering of the bridged fused ring system (see P-25.4.4). If there is a choice, low numbers are preferred (e.g., prop[1]eno rather than prop[2]eno).

Examples:

$-CH_2-$	methano (preferred prefix)
$-CH_2-CH_2-$	ethano (preferred prefix)
$-CH_2-CH_2-CH_2-$	propano (preferred prefix)
$-CH=CH-$	etheno (preferred prefix)
$-\overset{1}{C}H=\overset{2}{C}H-\overset{3}{C}H_2-$	prop[1]eno (preferred prefix)

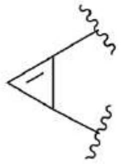
$-\overset{1}{C}H{=}\overset{2}{C}H{-}\overset{3}{C}H_2{-}\overset{4}{C}H_2{-}$ but[1]eno (preferred prefix)

$-\overset{1}{C}H_2{-}\overset{2}{C}H{=}\overset{3}{C}H{-}\overset{4}{C}H_2{-}$ but[2]eno (preferred prefix)

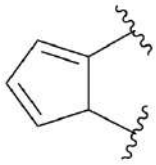
$-\overset{1}{C}H{=}\overset{2}{C}H{-}\overset{3}{C}H{=}\overset{4}{C}H{-}$ buta[1,3]dieno (preferred prefix)

P-25.4.2.1.2 A divalent monocyclic hydrocarbon bridge other than benzene is named by the same prefix as that used as a fusion prefix (P-25.3.2.2). To distinguish between these two, 'epi' is added in front of the name when used as a bridge prefix; the letter 'i' in the prefix 'epi' is elided before the letters 'i' and 'o' of the following term. [CAS uses the italicized prefix '*endo*'.] The bridge is assumed to have the maximum number of noncumulative double bonds consistent with its attachments to the fused ring system or to other bridges. The positions of the free valences of the bridge are indicated by locants in square brackets cited directly in front of the bridge name; these locants are not those used for bridge atoms in the final structure, for which see P-25.4.4. Locants for indicated hydrogen atoms, if present, are those for the final structure and are cited in front of the completed name (see P-25.4.3.4).

Examples:



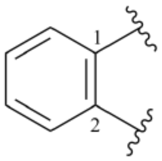
[1,3]epicyclopropa (preferred prefix)
['epicyclopropa' in ref. 4, FR 8.3.1(b)]



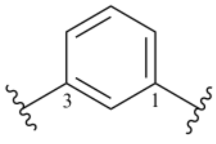
[1,2]epicyclopenta (preferred prefix)

P-25.4.2.1.3 Divalent cyclic hydrocarbon bridges not named in P-25.4.2.1.2 are named as a prefix derived from the corresponding hydrocarbon name by replacing the terminal letter 'e' by 'o'. If the name of the bridge is the same as the name of the fusion prefix, the bridge prefix is distinguished by the prefix 'epi-'. [CAS uses the italicized prefix '*endo*'.] The letter 'i' is elided if followed by a vowel. Locants for positions of free valences of the bridge and for indicated hydrogen, if necessary, are cited in the same way as described in section P-25.4.2.1.2.

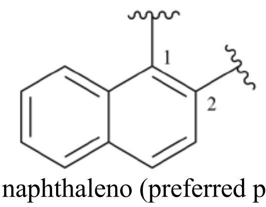
Examples:



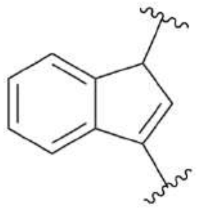
[1,2]benzeno (preferred prefix)
(not [1,2]epibenzo;
benzo is the name of a fusion prefix)



[1,3]benzeno (preferred prefix)
(not [1,3]epibenzo;
benzo is the name of a fusion prefix)



[1,2]naphthaleno (preferred prefix)
(not [1,2]epinaphtho;
naphtho is the name of a fusion prefix)



[1,3]epindeno (preferred prefix)
(not [1,3]indeno;
indeno is the name of a fusion prefix)

P-25.4.2.1.4 A divalent acyclic homogeneous heteroatom bridge is named by a prefix based either on a substitutive prefix or the name of the corresponding parent hydride. Bridge prefixes based on a substitutive prefix, in use today or formerly recommended, are distinguished by the prefix ‘epi’ (or ‘ep’ before the letter ‘i or ‘o’ of the following term). Bridge prefixes based on the name of a parent hydride are named in the same way as for acyclic hydrocarbon bridge prefixes (see P-25.4.2.1.1). Heteroatoms with nonstandard bonding numbers are described by the λ-convention (see P-14.1).

> The following names are now recommended as preselected (see P-12.2) bridge prefixes: ‘sulfano’, –S–;‘disulfano’, –SS–; ‘selano’, –Se–; ‘tellano’, –Te–; ‘azano‘, –NH–; ‘diazeno’, –N=N–; ‘epitriazano’, –NH-NH-NH–; and –NH-N=N–, ‘epitriaz[1]eno’. The bridge prefixes ‘epithio’, ‘epidithio’, ‘episeleno’, ‘epitelluro’, and ‘epimino’ [ref. 4, FR-8.3.1(d)] may be used in general nomenclature, as noted in the following examples.

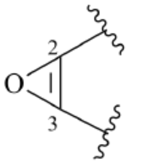
Examples:

–O–	epoxy (preselected prefix) (not epoxidano)
–O-O–	epidioxy (preselected prefix) (not epiperoxy)
–O-O-O–	epitrioxy [preselected prefix, see ref. 4, FR-8.3.1(d)] epitrioxidanediyl
–S–	sulfano (preselected prefix) epithio [see ref. 4, FR-8.3.1(d)]
–SH$_2$–	λ^4-sulfano (preselected prefix)
–S-S–	disulfano (preselected prefix) epidithio [see ref. 4, FR-8.3.1(d)]
–Se–	selano (preselected prefix) episeleno [see ref. 4, FR-8.3.1(d)]
–Te–	tellano (preselected prefix) epitelluro [see ref. 4, FR-8.3.1(d)]
–SiH$_2$–	silano (preselected prefix)
–SnH$_2$–	stannano (preselected prefix)
–NH–	azano (preselected prefix) epimino [see ref. 4, FR-8.3.1(d)] (not imino given in ref. 1, C-815.2)
–NH-NH–	diazano (preselected prefix) biimino (see ref. 1, B-15.1)
–N=N–	diazeno [preselected prefix; see ref. 4 FR-8.3.1(d)]) azo (see ref. 1, B-15.1)
–NH-NH-NH–	epitriazano (preselected prefix) (not triazano, which has been used for H$_2$N-NH-NH–, see C-942.3, ref. 1, which is triazan-1-yl in these recommendations, see P-68.3.1.4.1)

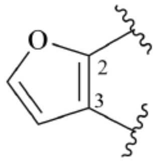
$-\overset{3}{\mathrm{N}}\mathrm{H}-\overset{2}{\mathrm{N}}=\overset{1}{\mathrm{N}}-$	epitriaz[1]eno (preselected prefix) (not triaz[1]eno, which has been used for H_2N-N=N–, see C-942.3, ref. 1, which is triaz-1-en-1-yl in these recommendations, see P-68.3.1.4.1) azimino (see ref. 1, B-15.1)
–PH–	phosphano (preselected prefix)
–BH–	borano (preselected prefix)

P-25.4.2.1.5 A divalent heterocyclic bridge is named as a prefix derived from the corresponding heterocyclic compound by adding a letter ‘o’ with elision of a final letter ‘e’ if present. If the heterocyclic system requires the citation of locants, these are given in square brackets in front of the name of the prefix. If the name of the bridge is the same as the fusion prefix, the bridge prefix is distinguished by the prefix ‘epi’ (or ‘ep’ before the letter ‘i’ or ‘o’ of the following term). [CAS uses the italicized prefix ‘*endo*’.] If indicated hydrogen is required for the bridge component, it is cited in front of the name of the complete bridged fused ring system and not in front of the name of the bridge itself (see P-25.7.1). For numbering of bridges, see P-25.4.4.

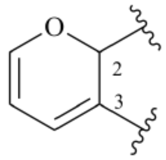
Examples:



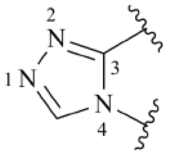
epoxireno (preferred prefix)



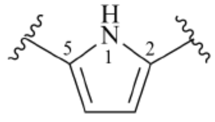
[2,3]furano (preferred prefix)
(not [2,3]epifurano;
nor [2,3]epifuro)



[2,3]epipyrano (preferred prefix)



[3,4]epi[1,2,4]triazolo (preferred prefix)



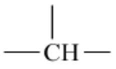
[2,5]epipyrrolo (preferred prefix)

P-25.4.2.2 Polyvalent bridges

P-25.4.2.2.1 A polyvalent bridge consisting of one atom (other than hydrogen) is named as a prefix based either on a substitutive prefix to which the prefix ‘epi’ is added as described in P-25.4.2.1.4 or by changing the ending ‘ano’ in the name of a divalent monoatomic bridge described in P-25.4.2.1.4 into ‘eno’, for example ‘metheno’ from ‘methano’. Polyvalent bridges are enclosed within parentheses in names of bridged fused systems; as a reminder, parentheses are placed around the names of the bridges themselves in the examples below. Where there is a choice, an attachment by a single bond, i.e., ‘yl’, is to the lower locant of a parent ring system. For ‘epi’, see P-25.4.2.1.4.

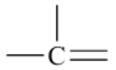
Examples:

–CH=	(metheno) (preferred prefix) (epimethanylylidene)



$-\overset{|}{C}H-$

(epimethanetriyl) (preferred prefix)
(methyno)

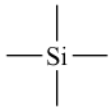


$-\overset{|}{C}=$

(epimethanediylylidene) (preferred prefix)

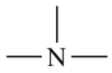
–N=

(azeno) (preselected prefix)
(epiazanylylidene)
(not ‘nitrilo’, see ref. 2, R-9.2.2)



$-\overset{|}{\underset{|}{Si}}-$

(episilanetetrayl) (preselected prefix)

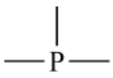


$-\overset{|}{N}-$

(epinitrilo) (preselected prefix)
epiazanetriyl [ref. 4, FR-8.3.2 (a)]
[not nitrilo]

–P=

(phospheno) (preselected prefix)
(epiphosphanylylidene) [ref. 4, FR-8.3.2 (a)]



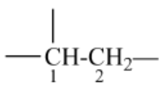
$-\overset{|}{P}-$

(epiphosphanetriyl) (preselected prefix)
[not phosphanetriyl, [ref. 4 FR-8.3.2 (a);
nor phosphinidyne]

P-25.4.2.2.2 A polyvalent polyatomic bridge is named as the polyvalent substituent group and enclosed in parentheses in names (as a reminder, parentheses are placed around the names of the bridges themselves in the examples below). If necessary, the positions of the free valences are indicated by appropriate locants cited directly in front of the associated ending. The suffix ‘ylidene’ is restricted to those cases in which there is a double bond between the bridge and the fused system. When there is a choice of numbering the bridge, preference is given to (a) the suffix ‘yl’, (b) the suffix ‘ylidene’, (c) double bonds. For ‘epi’, see P-25.4.2.1.4.

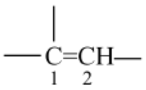
Examples:

$-CH_2-CH=$ (epiethanylylidene) (preferred prefix)



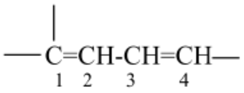
$-\overset{|}{\underset{1}{C}}H-\underset{2}{C}H_2-$

(epiethane[1,1,2]triyl) (preferred prefix)



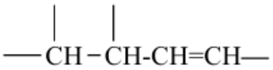
$-\overset{|}{\underset{1}{C}}=\underset{2}{C}H-$

(epiethene[1,1,2]triyl) (preferred prefix)



$-\overset{|}{\underset{1}{C}}=\underset{2}{C}H-\underset{3}{C}H=\underset{4}{C}H-$

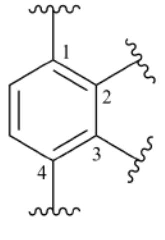
(epibuta[1,3]diene[1,1,4]triyl) (preferred prefix)



$-\overset{|}{C}H-\overset{|}{C}H-CH=CH-$

(epibut[3]ene[1,1,2,4]tetrayl) (preferred prefix)

=N-N= (epidiazanediylidene) (preselected prefix)



(epibenzene[1,2,3,4]tetrayl) (preferred prefix)

P-25.4.2.3 Composite bridges

P-25.4.2.3.1 Composite bridge names are formed by concatenating the names of two or more simple bridges. Unless cited first, the prefix ‘epi’ (or ‘ep’ before the letter ‘i’ or ‘o’ of the following term) is omitted. The prefixes are cited without elision in order starting from the senior prefix based on the following criteria applied in turn until a decision is reached.

(a) the simple bridge containing the heteroatom appearing first in the list: O > S > Se > Te > N > P > As > Sb > Bi > Si > Ge > Sn > Pb > B > Al > Ga > In > Tl;

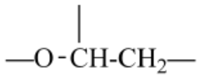
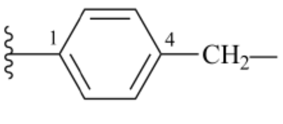
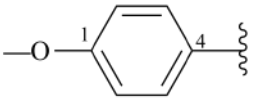
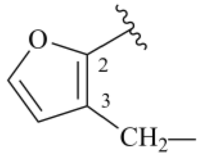
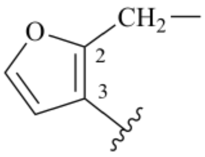
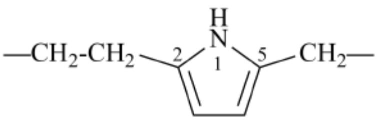
(b) the simple bridge containing the senior ring system;

(c) the simple bridge containing the longer acyclic chain;

(d) the simple bridge that occurs first in alphanumerical order.

P-25.4.2.3.2 Composite bridges are enclosed within parentheses in names of bridged fused compounds (as a reminder, parentheses are placed around the names of bridges themselves in the examples below). Locants for indicated hydrogen atoms required for a cyclic component of a composite bridge are cited in front of the name of the complete bridged fused ring system and not in front of the name of the bridge itself (see P-25.7.1). For numbering of bridges see P-25.4.4. If an acyclic bridge component requires internal numbering it is numbered in the direction implied by the bridge name.

Examples:

$-O-CH_2-$	(epoxymethano) (preferred prefix)
$-NH-CH_2-CH_2-$	(azanoethano) (preferred prefix)
$-O-S-O-$	(epoxysulfanooxy) (preselected prefix)
 $-O-\overset{\vert}{C}H-CH_2-$	(epoxyethane[1,1,2]triyl) (preferred prefix)
$-O-CH_2-CH<$	(epoxyethane[1,2,2]triyl) (preferred prefix)
	([1,4]benzenomethano) (preferred prefix)
	(epoxy[1,4]benzeno) (preferred prefix)
	([2,3]furanomethano) (preferred prefix)
	([3,2]furanomethano) (preferred prefix)
	[ethano([2,5]epipyrrolo)methano] (preferred prefix)
$-CH_2-O-CH=$	(methanooxymetheno) (preferred prefix)

P-25.4.3 Naming bridged fused ring systems

P-25.4.3.1 Citation of bridges
P-25.4.3.2 Attachment locants
P-25.4.3.3 Choice of attachment locants
P-25.4.3.4 Selection of bridges

P-25.4.3.1 Citation of bridges

If there is more than one bridge, they are cited in alphabetical order, unless one bridge is dependent on another. In that case, the dependent bridge is cited in front of all independent bridges. Two or more identical bridges are indicated by the numerical prefixes ‘di’, ‘tri’, etc. with simple bridges (P-25.4.1.4), or ‘bis’, ‘tris’, etc. with composite bridges (P-25.4.1.5) or if ‘di’, ‘tri’, etc. would be ambiguous. The locant pairs of identical bridges are separated by colons.

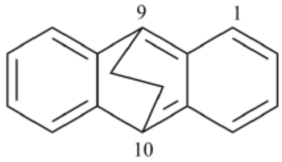
P-25.4.3.2 Attachment locants

The fused ring system to be bridged is numbered in the usual way. For selection of the fused ring to be bridged see P-25.4.3.4.2.

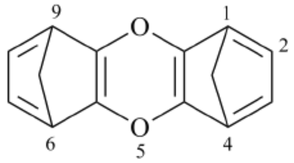
P-25.4.3.2.1 Divalent symmetric bridges

The locants of the positions on the fused ring system to which divalent symmetric bridges (are) attached are cited in numerical order in front of each bridge name.

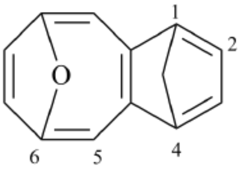
Examples:



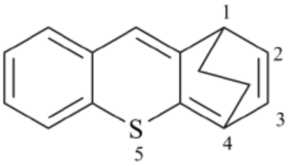
9,10-ethanoanthracene (PIN)



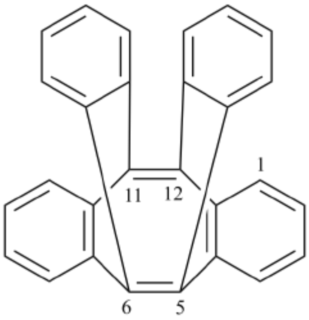
1,4:6,9-dimethanooxanthrene (PIN)
1,4:6,9-dimethanodibenzo[*b*,*e*][1,4]dioxine



6,9-epoxy-1,4-methanobenzo[8]annulene (PIN)



1*H*-1,4-ethanothioxanthene (PIN)

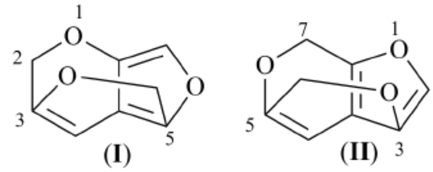


5,12:6,11-di[1,2]benzenodibenzo[*a*,*e*][8]annulene (PIN)

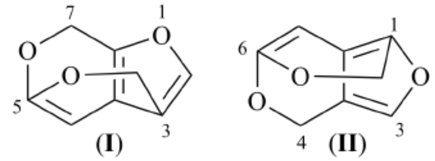
P-25.4.3.2.2 Polyvalent and composite bridges

Locants of the positions on the fused ring system to which polyvalent or composite bridges are attached are cited in the order expressed or implied by the name of the bridge. Methods of assigning locants for the free valences of bridges are given in section P-25.4.2. In the absence of specific locants, a single free valence (yl) is assigned a lower locant than a double free valence (ylidene). If there is a choice, locants are cited in numerical order. Indicated hydrogen atoms are cited at the front of the complete bridged fused ring name and not in front of names of the bridges themselves (P-25.7.1).

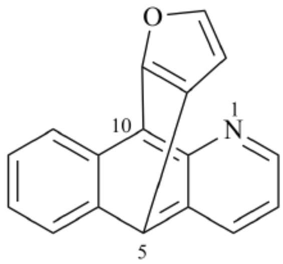
Examples:



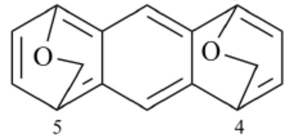
2*H*-3,5-(epoxymethano)furo[3,4-*b*]pyran (**I**) (PIN)
(not 7*H*-3,5-(epoxymethano)furo[2,3-*c*]pyran) (**II**)
[preferred ring system, see P-25.4.3.4.2 (d)]



7*H*-5,3-(epoxymethano)furo[2,3-*c*]pyran (**I**) (PIN)
(not 4*H*-6,1-(epoxymethano)furo[3,4-*c*]pyran (**II**)
[preferred ring system, see P-25.4.3.4.2 (d)]



10,5-[2,3]furanobenzo[*g*]quinoline (PIN)



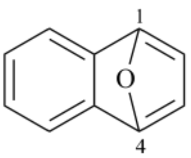
1,4:8,5-bis(epoxymethano)anthracene (PIN)

P-25.4.3.3 Choice of attachment locants

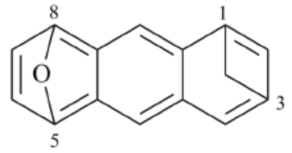
If there is a choice of attachment locants after the application of P-25.4.3.2, seniority is established in the following order:

(a) the lowest set of locants for all the bridge attachment points considered as a set;

Examples:



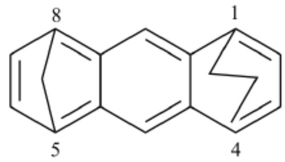
1,4-epoxynaphthalene (PIN)
(not 5,8-epoxynaphthalene)



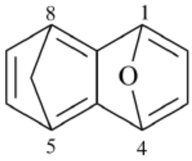
5,8-epoxy-1,3-methanoanthracene (PIN)
(not 1,4-epoxy-5,7-methanoanthracene;
the locant set 1,3,5,8 is lower than 1,4,5,7)

(b) lowest locants in the order of citation for the bridges;

Examples:



1,4-ethano-5,8-methanoanthracene (PIN)



1,4-epoxy-5,8-methanonaphthalene (PIN)

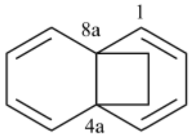
P-25.4.3.4 Selection of bridges

When a polycyclic ring system cannot be named completely as a fused ring system, possible ways for naming it as a bridged fused system are considered. Bridges are selected so that a recommended fused ring system as described in P-25.1 through P-25.3 is the parent fused ring system that is bridged.

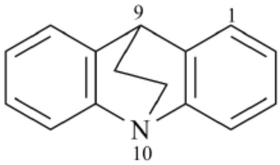
P-25.4.3.4.1 Naming of *ortho*- or *ortho*- and *peri*-fused systems

The ring system that remains after removal of the bridge(s) is named according to P-25.1 through P-25.3. The maximum number of noncumulative double bonds is assigned to the fused ring system after the insertion of the bridge. Thus, in allowing for the bonds of the bridge, the number of noncumulative double bonds and/or the need for indicated hydrogen may be different than in the parent ring system. If needed, indicated hydrogen is used to identify the specific isomer and is cited in front of the completed bridged fused ring name (see P-25.7.1.3.2).

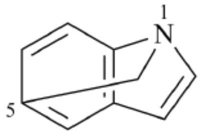
Examples:



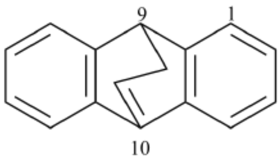
4a,8a-ethanonaphthalene (PIN)



9*H*-9,10-ethanoacridine (PIN)



1,5-methanoindole (PIN)



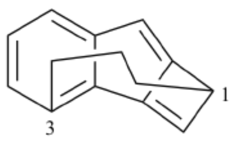
9*H*-9,10-(epiethanylylidene)anthracene
[not 9*H*-10,9-(epiethanylylidene)anthracene;
the ‘yl’ suffix is given preference for the low locant
of attachment to the ring system (see P-25.4.3.2.2)]

P-25.4.3.4.2 Selection of fused ring system to be bridged

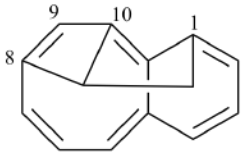
If there is a choice for selecting the fused ring system to be bridged, the criteria in the following list are applied in order until a complete decision is reached. Two structures might differ in the distribution of double bonds as described in P-25.4.3.4.1. Locants of the fused ring system where bridges are attached are then cited in front of the name of the bridge and in the same order as the locants for the free valences of the bridge (see P-25.4.3.2.2). The fused ring system, before bridging must:

(a) contain the maximum number of rings;

Example:



not



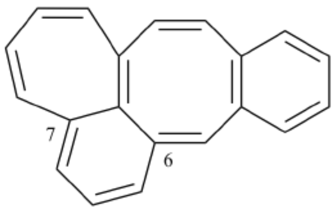
(**I**) (**II**)

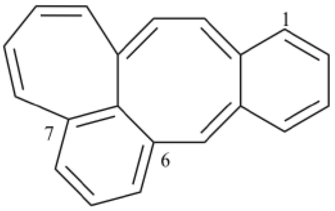
1*H*-1,3-propanocyclobuta[a]indene (**I**) (PIN)
[not 8,10,1-(epiethane[1,1,2]triyl)benzo[8]annulene(**II**)
(for order of ring attachment locants see P-25.4.3.2.2)

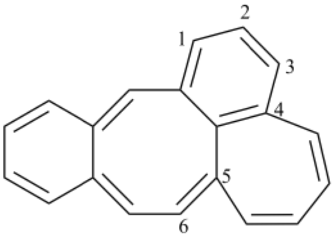
Explanation: the correct name has three rings in the fused ring system; the incorrect name has only two rings in the fused ring system.

(b) include the maximum number of skeletal atoms;

Example:





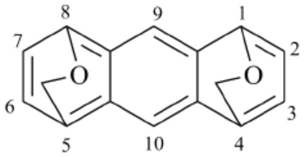


(**I**) (**II**) (**III**)

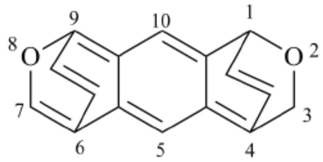
6,7-(epiprop[1]en[1]yl[3]ylidene)benzo[*a*]cyclohepta[e][8]annulene (**I**) (PIN)
[not 7,6-(epiprop[1]en[1]yl[3]ylidene)benzo[*a*]cyclohepta[*e*][8]annulene (**II**);
the 'yl' suffix is given the lower attachment point of the ring system (see P-25.4.3.2.2)
[not 4,5-buta[1,3]dienodibenzo[*a*,*d*][8]annulene (**III**);
the fused ring system benzo[*a*]cyclohepta[*e*][8]annulene has 17 atoms
whereas the fused ring system dibenzo[*a*,*d*][8]annulene has only 16 atoms]

(c) have the fewer heteroatoms in the fused ring system before bridging;

Example:



not

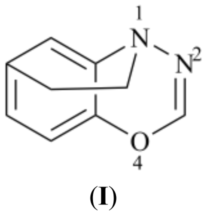


(**I**) (**II**)

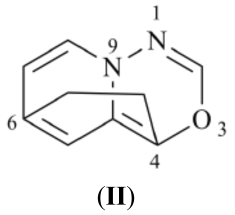
1,4:8,5-bis(epoxymethano)anthracene (**I**) (PIN) [not 1*H*,3*H*-1,4:6,9-bisethenobenzo[1,2-*c*:5,4-*c′*]dipyran (**II**);
zero heteroatoms in the fused ring system before bridging is fewer than two]

(d) consist of the most senior ring system, when the seniority order is applied to the parent fused ring system (see P-44.2);

Examples:

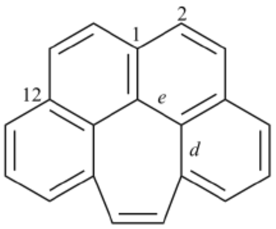


not

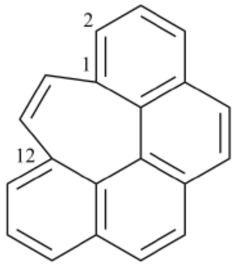


(**I**) (**II**)

1,7-ethano[4,1,2]benzoxadiazine (**I**) (PIN) [not 4,6-ethanopyrido[1,2-*d*][1,3,4]oxadiazine (**II**);
the locant set '1,2,4' for the heteroatoms in (**I**) is lower
than the locant set '1,3,9' in (**II**) (see P-14.3.5)]

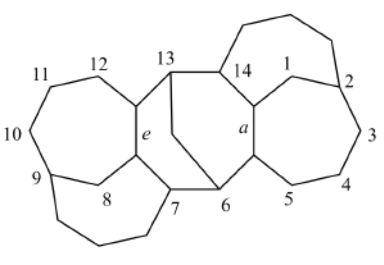


(**I**)

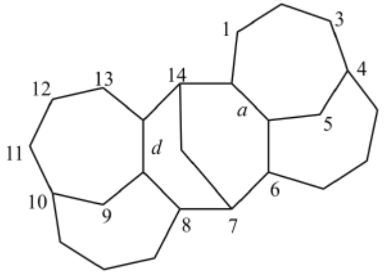


(**II**)

1,12-ethenobenzo[4,5]cyclohepta[1,2,3-*de*]naphthalene (**I**) (PIN)
{not 1,12-ethenobenzo[*c*]phenanthrene (**II**);
the ring size set ‘7,6,6,6’ in (**I**) is preferred
to the ring size set ‘6,6,6,6’ in (**II**)
[see P-25.3.2.4 (c) and P-44.2.2.2.3 (a)]}


11
12
13
14
1
2
10
e
a
3
9
8
7
6
5
4

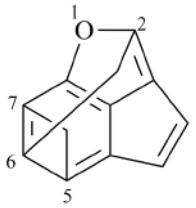
(**I**)


2
3
1
4
12
13
14
a
5
11
d
10
9
8
7
6

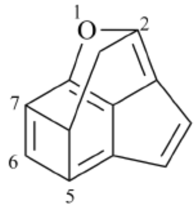
(**II**)

(e) have the minimum number of polyvalent bridges;

Examples:

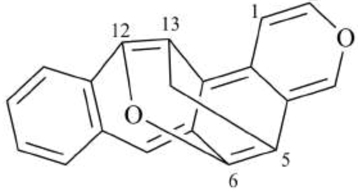


not

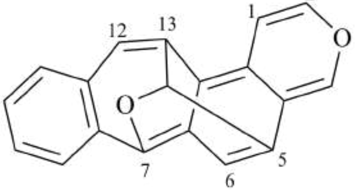


(**I**) (**II**)

2,6:5,7-dimethanoindeno[7,1-*bc*]furan (**I**) (PIN)
(for the order of ring attachment locants see P-25.4.3.2.2)
[not 5,7,2-(epiethane[1,1,2]triyl)indeno[7,1-*bc*]furan (**II**);
the PIN (**I**) has no polyvalent bridges; the incorrect name (**II**) has one polyvalent bridge]


12
13
1
2
O
O
6
5

not

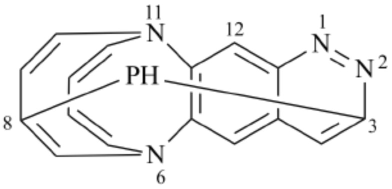

12
13
1
2
O
O
7
6
5

(**I**) (**II**)

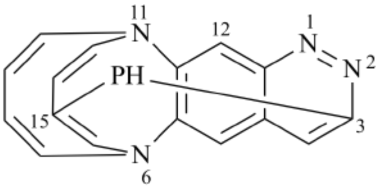
6,12-epoxy-5,13-methanobenzo[4,5]cyclohepta[1,2-*f*][2]benzopyran (**I**) (PIN)
6,12-epoxy-5,13-methanobenzo[4,5]cyclohepta[1,2-*f*]isochromene (**I**)
(for the order of ring attachment locants see P-25.4.3.2.2)
[not 7,5,13-(epoxymethanetriyl)benzo[4,5]cyclohepta[1,2-*f*]isochromene (**II**);
the PIN (**I**) has no polyvalent bridges; the incorrect name (**II**) has one polyvalent bridge]

(f) have the minimum number of dependent bridges;

Example:


11
N
12
1
N
N
2
PH
8
3
N
6

not

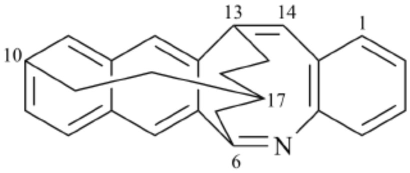

11
N
12
1
N
N
2
PH
15
3
N
6

(**I**) (**II**)

6,11-buta[1,3]dieno-3,8-phosphano[1,4]diazocino[2,3-*g*]cinnoline (**I**) (PIN)
[not 3,15-phosphano-6,11-buta[1,3]dieno[1,4]diazocino[2,3-*g*]cinnoline (**II**);
the PIN (**I**) has no dependent bridges; the incorrect name (**II**) has one dependent bridge]

(g) have the minimum number of atoms in dependent bridges;

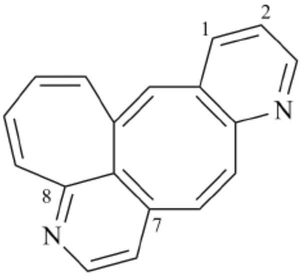
Example:



6,17-methano-10,13-pentanonaphtho[2,3-*c*][1]benzazocine (PIN)
[not 13,17-ethano-6,10-butanonaphtho[2,3-*c*][1]benzazocine)
nor 10,17-ethano-6,13-butanonaphtho[2,3-*c*][1]benzazocine);
the PIN has only one atom in a dependent bridge]

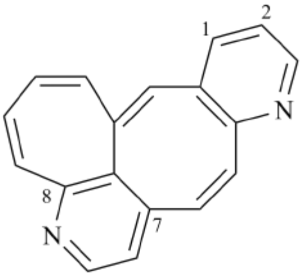
(h) have the maximum number of divalent bridges; thus 'diyl' is senior to 'ylylidene', 'triyl', 'diylidene', 'diylylidene', or 'tetrayl', etc. Similarly 'ylylidene' is senior to 'triyl', etc.

Example:



(**I**)

not

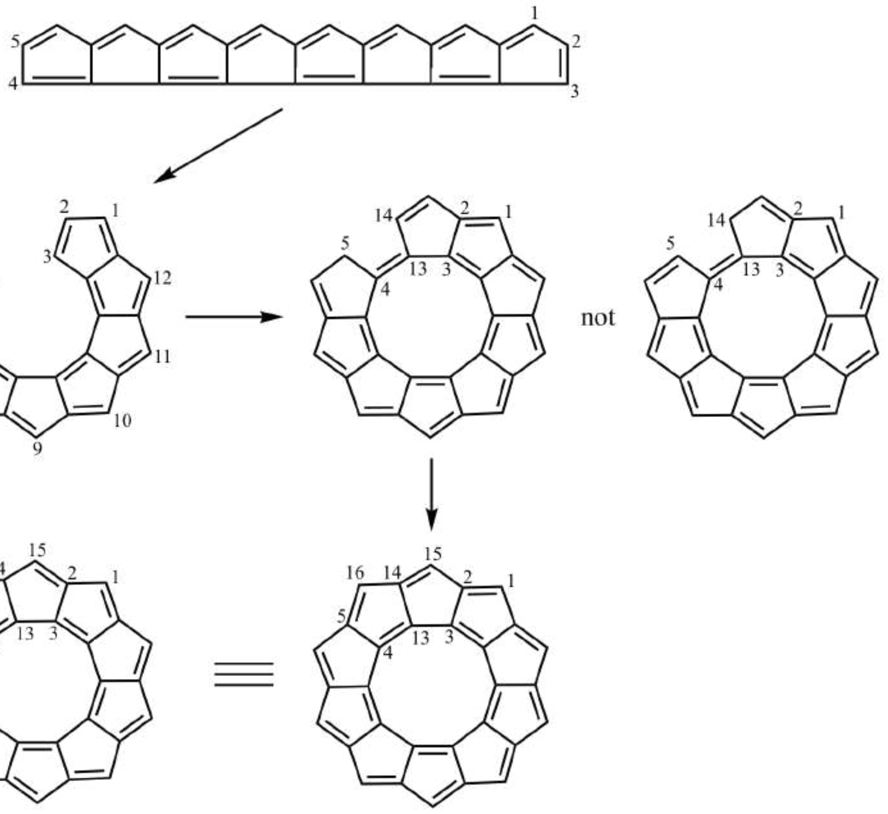


(**II**)

8,7-(azenoepietheno)cyclohepta[4,5]cycloocta[1,2-*b*]pyridine (**I**) (PIN)
[not 8,7-(azenoepiethanediylidene)cyclohepta[4,5]cycloocta[1,2-b]pyridine (**II**);
the PIN has a composite bridge consisting of a trivalent bridge and a divalent bridge whereas
the incorrect name contains a composite bridge consisting of a trivalent bridge and a tetravalent bridge]

(i) have the lowest locants at the location of bridges, first for independent bridges then dependent bridges;

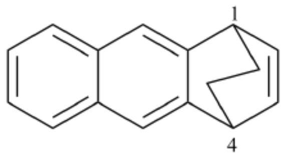
Example:



14,5-(metheno)-3,2,4-(epiprop[2]en[1,3]diyl[1]ylidene)dicyclopenta[*f*,*f*′]pentaleno[1,2-*a*:6,5-*a*′]dipentalene (PIN)
the locants set for the independent bridge ‘3,2,4’ is the lowest;
the locant for single bond attachment of metheno bridge is cited first.
[not 5,14-(metheno)-3,4,2-(epipropan[1]yl[1,3]diylidene)dicyclopenta[*f*,*f*′]]pentaleno[1,2-*a*:6,5-*a*′]dipentalene;
not 14,5-(metheno)-4,2,3-(epiprop[2]en[1,3]diyl[1]ylidene)dicyclopenta[*f*,*f*′]]pentaleno[1,2-*a*:6,5-*a*′]dipentalene;
not 5,14-(metheno)-4,3,2-(epipropan[1]yl[1,3]diylidene)dicyclopenta[*f*,*f*′]]pentaleno[1,2-*a*:6,5-*a*′]dipentalene;
(the locants ‘3,2,4’ for independent bridge is lower than ‘3,4,2’, ‘4,2,3’ and ‘4,3,2’]

(j) have the maximum number of noncumulative double bonds in the parent ring system;

Example:

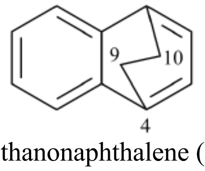


1,4-dihydro-1,4-ethanoanthracene (PIN)
(not 1,2,3,4-tetrahydro-1,4-ethenoanthracene)

P-25.4.4 Numbering of bridge atoms

Bridge atoms are numbered continuing from the highest locant of the fused ring system. If there is more than one bridge atom (excluding hydrogen) the numbering starts at the end of the chain or ring atom connected to the bridgehead of the fused ring system having the highest locant. With composite bridges, each component is completely numbered before the next component. Fusion atoms in fused ring bridges are numbered in accordance with P-25.3.3.1.1.

Example:



1,4-ethanonaphthalene (PIN)

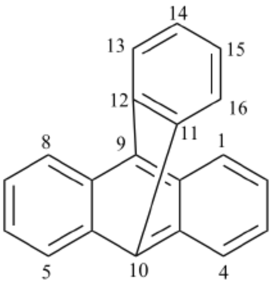
P-25.4.4.1 When there is a choice of locants, lowest locants are assigned according to the following criteria, in order, until a definitive decision is reached:

(a) low locants for heteroatoms;

(b) low locants for bridgehead atoms within a bridge;

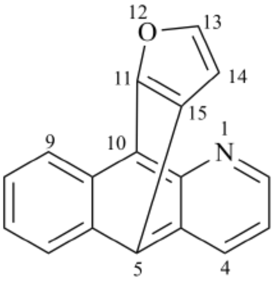
The remaining atoms (excluding hydrogen) are then numbered consecutively.

Examples:



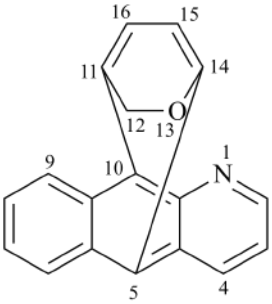
14
13
15
12
16
11
8
9
1
5
10
4

9,10-[1,2]benzenoanthracene (PIN)



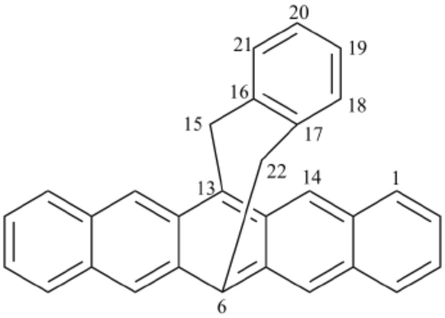
12
O
13
11
14
15
1
9
10
N
5
4

10,5-[2,3]furanobenzo[*g*]quinoline (PIN)



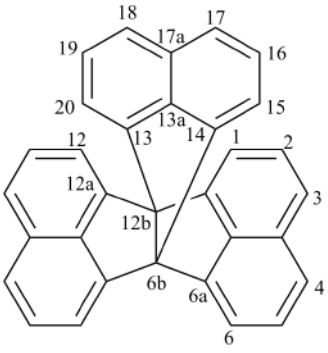
16
15
11
14
O
12
13
1
9
10
N
5
4

12*H*-5,10-[2,5]epipyranobenzo[*g*]quinoline (PIN)



20
21
19
16
18
15
17
22
14
1
13
6

6,13-(methano[1,2]benzenomethano)pentacene (PIN)



18
17
17a
19
16
20
13a
15
12
13
14
1
2
12a
3
12b
6b
4
6a
6

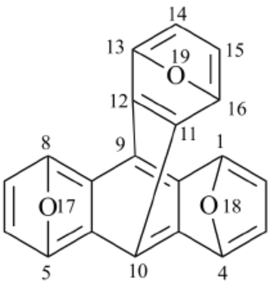
6b,12b-[1,8]naphthalenoacenaphthyleno[1,2-*a*]acenaphthylene (PIN)

Note: Locants 13a and 17a are generated in the same way as fusion locants for nonbridged fused ring systems, see P-25.3.3.1.1.

P-25.4.5 Order for numbering bridges

P-25.4.5.1 Independent bridges are numbered before dependent bridges.

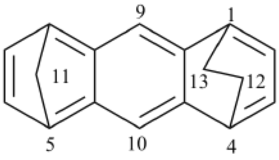
Example:



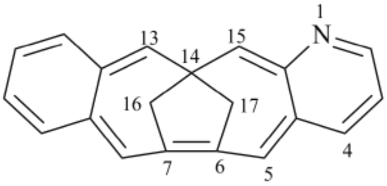
13,16-epoxy-1,4:5,8-diepoxy-9,10-[1,2]benzenoanthracene (PIN)
Note: Dependent bridges are cited before independent bridges but are numbered after them, see P-25.4.3.1.

P-25.4.5.2 If there is more than one bridge of the same type (dependent or independent), seniority is given to the bridge attached to the bridgehead with the higher locant at the first point of difference.

Examples



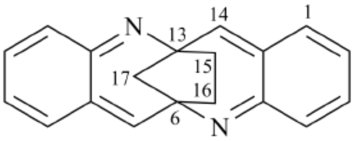
1,4-ethano-5,8-methanoanthracene (PIN)



6,14:7,14-dimethanobenzo[7,8]cycloundeca[1,2-*b*]pyridine (PIN)

P-25.4.5.3 If two bridges are attached to the same bridgehead atoms, they are numbered in accordance with their order of citation.

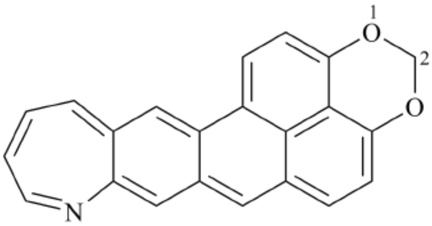
Example:



6,13-ethano-6,13-methanodibenzo[*b*,*g*][1,6]diazecine (PIN)

P-25.5 LIMITATIONS OF FUSION NOMENCLATURE: THREE COMPONENTS *ORTHO*- AND *PERI*-FUSED TOGETHER

The fusion principles described in P-25.1 through P-25.3 apply only between pairs of components. It is not possible by these principles to name a system in which a third component is *ortho*- and *peri*-fused to two components that are themselves *ortho*- or *ortho*- and *peri*-fused together. It is important to recall that benzo heterocycles are considered as one component, thus permitting the construction of names that would not otherwise be possible.



2*H*-[1,3]benzodioxino[6′,5′,4′:10,5,6]anthra[2,3-*b*]azepine (PIN)
Note: A normal fusion name is not possible when the four components azepine, anthracene, 1,3-dioxine and benzene are treated individually; therefore, the use of a benzo name component is necessary; 1-benzazepine cannot be the parent ring because this would require breaking of the attached component having a retained name, anthra, which is not allowed, see P-25.3.5.

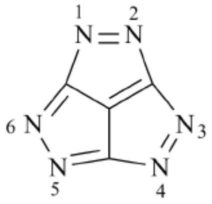
When a third component is *ortho*- and *peri*-fused to two components that are themselves *ortho*- or *ortho*- and *peri*-fused together, the following procedures are applied in order until a name can be formed.

P-25.5.1 Skeletal replacement (‘a’) nomenclature

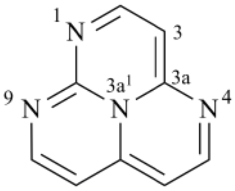
P-25.5.1.1 If the corresponding hydrocarbon fused ring system can be named by fusion principles or has a retained name, then heteroatoms are identified by skeletal replacement ('a') nomenclature using the appropriate 'a' prefixes (see P-22.2.3). The numbering of the fused hydrocarbon system is not altered by the 'a' prefixes.

When the fusion principles discussed in P-25.1 through P-25.3 do apply, no skeletal replacement ('a') name is recommended. The procedure is valid only for cases described in P-25.5.

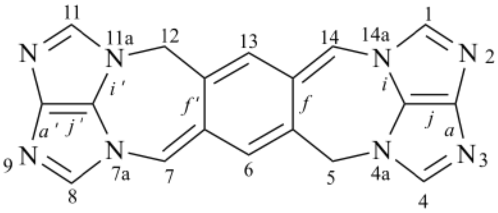
Examples:



1,2,3,4,5,6-hexaazacyclopenta[*cd*]pentalene (PIN)



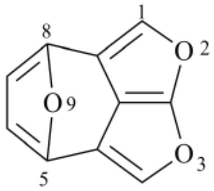
1,3a^1,4,9-tetraazaphenalene (PIN)



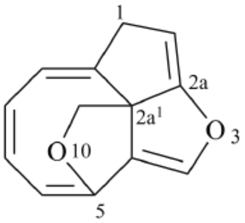
5*H*,12*H*-2,3,4a,7a,9,10,11a,14a-octaazadicyclopenta[*ij*:*i′j′*]benzo[1,2-*f*:4,5-*f′*]diazulene (PIN)

P-25.5.1.2 If the fused ring system can only be named using skeletal ('a') replacement nomenclature, any heteroatoms in bridge are also named using skeletal replacement ('a') nomenclature. The replacement terms are cited at the front of the corresponding hydrocarbon bridged fused ring system.

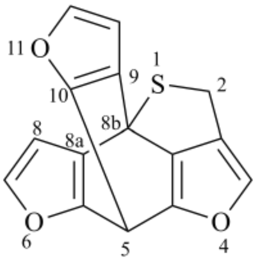
Examples:



2,3,9-trioxa-5,8-methanocyclopenta[*cd*]azulene (PIN)



1*H*-3,10-dioxa-2a^1,5-ethanocycloocta[*cd*]pentalene (PIN)

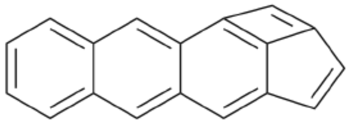


2*H*,5*H*-4,6,11-trioxa-1-thia-5,8b-[1,2]epicyclopentacyclopenta[*cd*]-*s*-indacene (PIN)

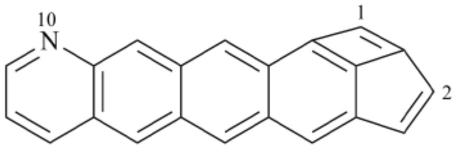
P-25.5.2 Selection of a less senior hydrocarbon parent component

A less preferred hydrocarbon parent component is selected that will permit a fusion name. Second and third choice parent components are chosen according to the seniority order for selecting the senior parent component (see P-25.3.2.4).

Examples:



cyclobuta[1,7]indeno[5,6-*b*]naphthalene (PIN)
(anthracene cannot be selected as senior parent component;
naphthalene, not indene, is next in seniority order for selection as a parent component)

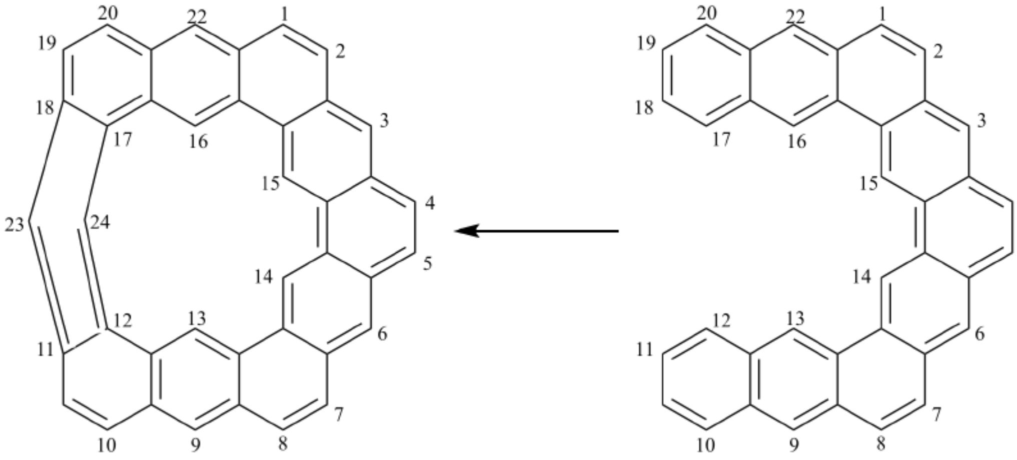


10-azacyclobuta[1,7]indeno[5,6-*b*]anthracene (PIN)
[neither quinoline nor pyridine can be used as the senior parent component because
neither naphthalene nor anthracene, respectively, can be used as the senior attached component;
therefore ‘a’ nomenclature must be used (see P-25.5.1) and since the preferred hydrocarbon tetracene cannot be used,
the next senior component, anthracene, is chosen as the parent component]

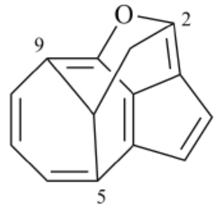
P-25.5.3 Use of bridging nomenclature

A bridged fused system (see Section P-25.4) is used to generate names for structures that cannot be named by normal fusion nomenclature. A fused system is first envisaged; additional rings are created by using bridges.

Examples:



12,19:13,18-di(metheno)dinaphtho[2,3-*a*:2′,3′-*o*]pentaphene (PIN)



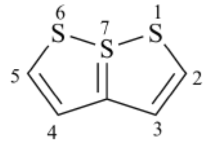
1-oxa-5,9,2-(epiethane[1,1,2]triyl)cycloocta[*cd*]pentalene (PIN)

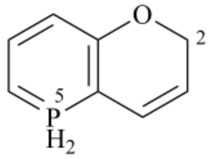
P-25.6 FUSED RING SYSTEMS WITH SKELETAL ATOMS WITH NONSTANDARD BONDING NUMBERS

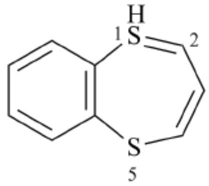
The λ-convention is used to describe atoms with nonstandard bonding numbers (ref. 13) in fused ring systems. The symbol λ^n is used, where ‘*n*’ is the bonding number of the atoms; it is cited immediately after the locant denoting the atom having the nonstandard bonding number. The symbol *H*, denoting indicated hydrogen atom(s) with the appropriate locant(s), if present, is cited at the front of the complete name.

The λ symbol is used with all ring systems described in this section with retained and fusion names, bi- and polyalicyclic as well as heterocycles formed by skeletal replacement (‘a’) nomenclature, as described above in P-25.5.1. Atoms with nonstandard bonding numbers in fused ring systems are indicated only in the complete ring system, not in component rings. Names and numbering are unchanged, unless a choice must be made between two otherwise equivalent atoms; in which case, low locants are attributed to atoms with the higher bonding numbers, for example λ^6 before λ^4.

Examples:

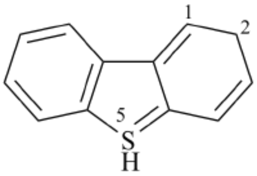

7λ^4-[1,2]dithiolo[5,1-*e*][1,2]dithiole (PIN)

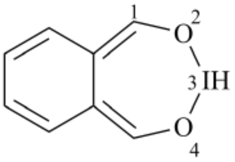

2*H*-5λ^5-phosphinino[3,2-*b*]pyran (PIN)

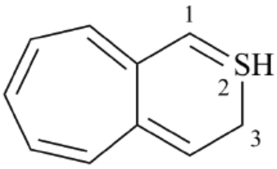

1λ^4,5-benzodithiepine (PIN)

After the maximum number of noncumulative double bonds has been assigned, any ring atom with a bonding number of three or higher connected to adjacent ring atoms by single bonds only and carrying one or more hydrogen atoms, is designated by the indicated hydrogen symbol *H*. If there is a choice, such ring atoms are selected for low locants.

Examples:


2*H*-5λ^4-dibenzo[*b*,*d*]thiophene (PIN)


3*H*-3λ^3,2,4-benziodadioxepine (PIN)


3*H*-2λ^4-cyclohepta[*c*]thiopyran (PIN)

P-25.7 DOUBLE BONDS, INDICATED HYDROGEN, AND THE Δ-CONVENTION

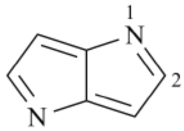
The treatment of double bonds is formalized in fusion nomenclature. A maximum of noncumulative double bonds must be present in fused and bridged fused systems. When hydrogen atoms are in excess at specific positions, they are denoted in names by indicated hydrogen atom(s). However, the presence of cumulative formal double bonds is also possible. This feature is expressed by the δ-convention (delta-Convention) (see ref. 24). These two aspects of fused and bridged fused systems are described in this Section.

P-25.7.1 Indicated hydrogen

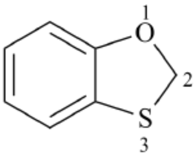
P-25.7.1.1 Maximum number of noncumulative double bonds

The names of polycyclic fused ring systems are considered to correspond to the structure with the maximum number of noncumulative double bonds consistent with the appropriate bonding number of the skeletal atoms. To achieve this result, components are fused together and noncumulative double bonds are introduced into the completed fused system. Hydrogen atoms not attached to atoms connected by double bonds are denoted as indicated hydrogen atom(s).

Examples:



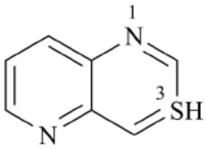
pyrrolo[3,2-*b*]pyrrole (PIN)



2*H*-1,3-benzoxathiole (PIN)

If atoms with nonstandard bonding numbers are present, they must be indicated using the λ-convention (and if necessary the δ-convention). The stated bonding number is used in assigning noncumulative double bonds.

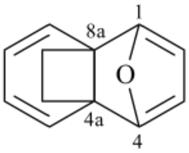
Example:



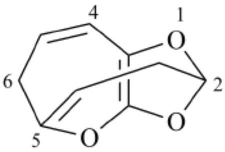
3λ^4-pyrido[3,2-*d*][1,3]thiazine (PIN)

In bridged fused systems, the distribution of noncumulative double bonds in the parent fused ring system is accomplished after allowance has been made for the bonds existing between the bridge(s) and the fused ring system. Rings that are part of a bridge are treated separately, after consideration of the free valences of the bridge.

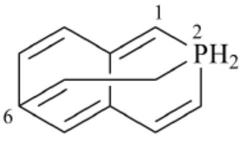
Examples:



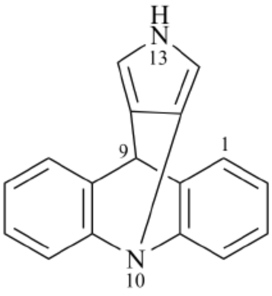
1,4-epoxy-4a,8a-ethanonaphthalene (PIN)



2*H*,6*H*-2,5-(epiethanylylidene)[1,3]dioxolo[4,5-*b*]oxepine (PIN)



2*H*-2λ^5-2,6-(epiethanylylidene)isophosphinoline (PIN)

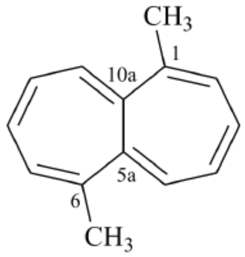


9*H*,13*H*-9,10-[3,4]epipyrroloacridine (PIN)

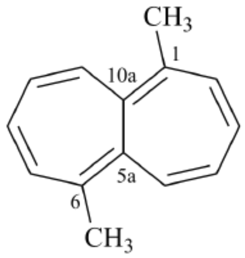
P-25.7.1.2 Localized double bonds

If it is necessary to identify isomers that differ only by virtue of the location of localized double bonds, this differentiation is indicated by the use of the Greek letter Δ. The locant cited corresponds to the first cited locant of the localized double bond.

Examples:



1,6-dimethyl-Δ^1-heptalene (PIN)



1,6-dimethyl-$\Delta^{1(10a)}$-heptalene (PIN)

P-25.7.1.3 Citation of indicated hydrogen

P-25.7.1.3.1 When a name applies equally to two or more isomeric systems with the maximum number of noncumulative double bonds and when the name can be made specific by indicating the position of one or more hydrogen atoms in the structure, this specifically is accomplished by adding to the name the italicized symbol *H* for each of these hydrogen atoms, preceded by the appropriate locant(s).

In preferred IUPAC names, all indicated hydrogen atoms must be cited when the names are constructed in accordance with the principles of fusion nomenclature

In general IUPAC nomenclature, omission of indicated hydrogen atoms is permitted in some parent fused ring systems, when unsubstituted, for example indene rather than 1*H*-indene, but 1*H*-indene-3-carboxylic acid. Omission of indicated hydrogen in general nomenclature is permitted in the following ring systems:

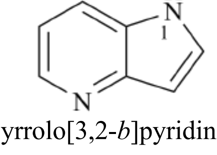
fluorene	9*H*
indene	1*H*
phenalene	1*H*
indazole	1*H*
indole	1*H*
isochromene (and chalcogen analogues)	1*H*
isoindole	2*H*
perimidine	1*H*
purine	7*H*
pyrrole	1*H*
xanthene	9*H*

Omission of indicated hydrogen is also permitted in general nomenclature if no ambiguity would result, for example 1,3-benzodioxole, rather than 2*H*-1,3-benzodioxole.

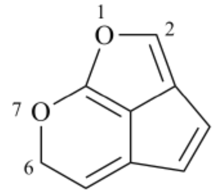
P-25.7.1.3.2 Indicated hydrogen with *ortho*-, and *ortho* and *peri*-fused systems

Indicated hydrogen is identified by the locant of the relevant position and cited at the front of the names of the whole ring system, including replacement terms, if any.

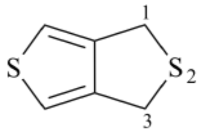
Examples:



1*H*-pyrrolo[3,2-*b*]pyridine (PIN)



6*H*-1,7-dioxacyclopenta[*cd*]indene (PIN)



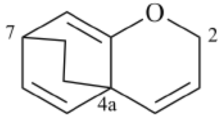
1*H*,3*H*-thieno[3,4-*c*]thiophene (PIN)

P-25.7.1.3.3 Indicated hydrogen with bridged fused ring systems

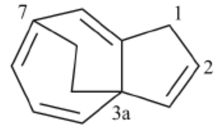
All indicated hydrogen atoms are indicated at the front of the complete name.

Note: Citation of indicated hydrogen in bridged fused ring systems in this manner is completely consistent with its citation for spiro atoms (see P-24.3.2) and ring assemblies (see P-28.2.3).

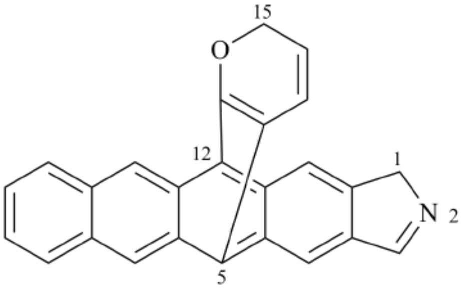
Examples:



2*H*,7*H*-4a,7-ethano-1-benzopyran (PIN)
2*H*,7*H*-4a,7-ethanochromene



1*H*-3a,7-ethanoazulene (PIN)

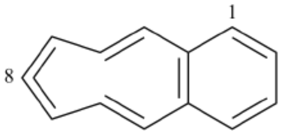


1*H*,15*H*-12,5-[2,3]epipyranoanthra[2,3-*f*]isoindole (PIN)

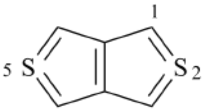
P-25.7.2 The δ-convention

The presence of contiguous formal double bonds at a skeletal atom in a cyclic parent hydride whose name normally implies the maximum number of noncumulative double bonds is described by the symbol δ^c, where '*c*' is the number of double bonds directly attached to the identified atom (see ref. 24). The δ^c symbol is cited immediately after an expressed locant for the skeletal atom in the name of the compound and follows the λ^n symbol, if present.

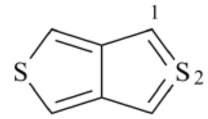
Examples:



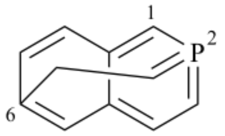
8δ^2-benzo[9]annulene (PIN)



2$\lambda^4\delta^2$,5$\lambda^4\delta^2$-thieno[3,4-*c*]thiophene (PIN)



$2\lambda^4\delta^2$-thieno[3,4-*c*]thiophene (PIN)



$2\lambda^5\delta^2$-6,2-(epiethanylylidene)isophosphinoline (PIN)

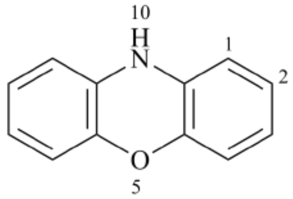
P-25.8 PARENT COMPONENTS IN DECREASING ORDER OF SENIORITY (partial lists)

In this subsection rings and ring systems are listed in decreasing order of seniority for selection as a parent component. The first list contains heterocyclic parent components, the second hydrocarbon parent components.

P-25.8.1 Partial list of heterocyclic parent components in decreasing order of seniority

The following list contains parent heterocycles arranged in decreasing order of seniority for selection as the parent component for fusion names. Ring systems containing Hg as given in ref. 4 are not included in these recommendations.

The parent heterocycles are arranged by ring analysis, i.e., in decreasing order of number rings, ring size, and in accordance with the priority given to heteroatoms, N, O, S, Se.



10*H*-phenoxazine

Note 1: Indicated hydrogen atoms are not shown in this kind of listing.

Note 2: The seniority order given below is used to select parent components in fusion nomenclature.

Note 3: In the order of seniority used by CAS quinolizine precedes quinoline and isoquinoline; and indolizine preceeds indole and isoindole.

phenoxazine	C_4NO-C_6-C_6	
phenothiazine	C_4NS-C_6-C_6	
phenoselenazine	C_4NSe-C_6-C_6	
phenotellurazine	C_4NTe-C_6-C_6	
phenazaphosphinine	C_4NP-C_6-C_6	
phenazarsinine	C_4NAs-C_6-C_6	
phenazine	C_4N_2-C_6-C_6	
phenanthroline	C_5N-C_5N-C_6	(in accordance with the positions of nitrogen atoms, in decreasing order of seniority: 1,7; 1,8; 1,9; 1,10; 2,7; 2,8; 2,9; 3,7; 3,8; 4,7)
perimidine	C_4N_2-C_6-C_6	
acridine	C_5N-C_6-C_6	
phenanthridine	C_5N-C_6-C_6	
carbazole	C_4N-C_6-C_6	
pteridine	C_4N_2-C_4N_2	
cinnoline	C_4N_2-C_6	
quinazoline	C_4N_2-C_6	
quinoxaline	C_4N_2-C_6	
1,5-naphthyridine	C_5N-C_5N	
1,6-naphthyridine	C_5N-C_5N	
1,7-naphthyridine	C_5N-C_5N	
1,8-naphthyridine	C_5N-C_5N	
phthalazine	C_5N-C_6	

2,6-naphthyridine	C_5N-C_5N
2,7-naphthyridine	C_5N-C_5N
quinoline	C_5N-C_6
isoquinoline	C_5N-C_6
quinolizine	C_5N-C_5N
purine	C_3N_2-C_4N_2
indazole	C_3N_2-C_6
indole	C_4N-C_6
isoindole	C_4N-C_6
indolizine	C_4N-C_5N
pyrrolizine	C_4N-C_4N

Seven-membered heterocyclic rings or larger with at least one nitrogen atom, for example azepine

Six-membered heterocyclic rings with at least three heteroatoms including at least one nitrogen atom, for example 1,3,5-oxadiazine

Six-membered heterocyclic rings with at least one nitrogen atom and a different heteroatom, for example 1,2-thiazine

pyridazine	C_4N_2
pyrimidine	C_4N_2
pyrazine	C_4N_2
pyridine	C_5N

Five-membered heterocyclic rings with at least three heteroatoms, including at least one nitrogen atom, for example 1,2,5-oxadiazole (formerly called furazan)

Five-membered heterocyclic rings with one nitrogen atom and a different heteroatom, for example 1,2-oxazole

pyrazole	C_3N_2
imidazole	C_3N_2
pyrrole	C_4N

Four- or three-membered heterocyclic rings with at least one nitrogen atom, for example azirene

Heterocyclic ring with halogen atom, but no nitrogen atom, for example 1λ^3-1,2-iodoxole

phenoxathiine	C_4OS-C_6-C_6
phenoxaselenine	C_4OSe-C_6-C_6
phenoxatellurine	C_4OTe-C_6-C_6
phenoxaphosphinine	C_4OP-C_6-C_6
phenoxarsinine	C_4OAs-C_6-C_6
phenoxastibinine	C_4OSb-C_6-C_6
oxanthrene	C_4O_2-C_6-C_6
xanthene	C_5O-C_6-C_6
1-benzopyran	C_5O-C_6
2-benzopyran	C_5O-C_6

Seven-membered heterocyclic ring or larger with at least one oxygen atom (no nitrogen atom), for example oxepine

Six-membered heterocyclic ring with two or more heteroatoms, at least one of which is oxygen, for example 1,4-dioxine

pyran	C_5O

Five-membered heterocyclic ring with two or more heteroatoms, one of which is oxygen (no nitrogen atom), for example 1,3-dioxole

furan	C_4O

Four- or three-membered heterocyclic ring with at least one oxygen atom (no nitrogen atom), for example oxirene

phenothiarsinine	C_4SAs-C_6-C_6
thianthrene	C_4S_2-C_6-C_6
thioxanthene	C_4S-C_6-C_6
1-benzothiopyran	C_5S-C_6
2-benzothiopyran	C_5S-C_6

Heteromonocyclic ring with at least one sulfur atom (no N or O atoms), for example thiopyran, C_5S

thiophene	C_4S
selenanthrene	C_4Se_2-C_6-C_6

selenoxanthene	C_5Se-C_6-C_6
1-benzoselenopyran	C_5Se-C_6
2-benzoselenopyran	C_5Se-C_6

Heteromonocyclic ring with at least one selenium atom (no N, O or S atoms), for example selenopyran, C_5Se

selenophene	C_4Se
telluranthrene	C_4Te_2-C_6-C_6
telluroxanthene	C_5Te-C_6-C_6
1-benzotelluropyran	C_5Te-C_6
2-benzotelluropyran	C_5Te-C_6

Heteromonocyclic ring with at least one tellurium atom (no N, O, S, or Se atoms), for example telluropyran, C_5Te

tellurophene	C_4Te
phosphanthrene	C_4P_2-C_6
acridophosphine	C_5P-C_6-C_6
phosphanthridine	C_5P-C_6-C_6
phosphinoline	C_5P-C_6-C_6
isophosphinoline	C_5P-C_6
phosphinolizine	C_5P-C_6
phosphindole	C_4P-C_6
isophosphindole	C_4P-C_6
phosphindolizine	C_4P-C_5P

Heteromonocyclic ring with at least one phosphorus atom (no N, O, S, Se, or Te atoms)

arsanthrene	C_4As_2-C_6
acridarsine	C_5As-C_6-C_6
arsanthridine	C_5As-C_6-C_6
arsinoline	C_5As-C_6-C_6
isoarsinoline	C_5As-C_6
arsinolizine	C_5As-C_6
arsindole	C_4As-C_6
isoarsindole	C_4As-C_6
arsindolizine	C_4As-C_5As

Heteromonocyclic ring with at least one arsenic atom, and Sb, Bi, Si, Ge, Sn, Pb, B, Al, Ga, In, and Tl as possible heteroatoms.

silanthrene	C_4Si_2-C_6-C_6
boranthrene	C_4B_2-C_6-C_6

P-25.8.2 Partial list of hydrocarbon parent components in decreasing order of seniority

Parent components are arranged:

(1) in decreasing order of number of rings;

(2) in decreasing order of ring size;

(3) in decreasing order of senior orientation;

(4) for aceanthrylene and acephenanthrylene, in increasing order of fusion atom locants;

(5) in the order of seniority used by CAS the indacenes precede biphenylene.

ovalene	$C_6C_6C_6C_6C_6C_6C_6C_6C_6C_6$
octaphenylene	$C_{16}C_6C_6C_6C_6C_6C_6C_6C_6$
tetranaphthylene	$C_8C_6C_6C_6C_6C_6C_6C_6C_6$
nonacene	$C_6C_6C_6C_6C_6C_6C_6C_6C_6$
nonaphene	$C_6C_6C_6C_6C_6C_6C_6C_6C_6$
nonahelicene	$C_6C_6C_6C_6C_6C_6C_6C_6C_6$
octacene	$C_6C_6C_6C_6C_6C_6C_6C_6$

octaphene	$C_6C_6C_6C_6C_6C_6C_6C_6$
pyranthrene	$C_6C_6C_6C_6C_6C_6C_6C_6$
octahelicene	$C_6C_6C_6$-$C_6C_6C_6C_6C_6$
hexaphenylene	$C_{12}C_6C_6C_6C_6C_6C_6$
heptacene	$C_6C_6C_6C_6C_6C_6C_6$
heptaphene	$C_6C_6C_6C_6C_6C_6C_6$
trinaphthylene	$C_6C_6C_6C_6C_6C_6C_6$
coronene	$C_6C_6C_6C_6C_6C_6C_6$
heptahelicene	$C_6C_6C_6C_6C_6C_6C_6$
rubicene	$C_6C_6C_6C_6C_6C_5C_5$
hexacene	$C_6C_6C_6C_6C_6C_6$
hexaphene	$C_6C_6C_6C_6C_6C_6$
hexahelicene	$C_6C_6C_6C_6C_6C_6$
tetraphenylene	$C_8C_6C_6C_6C_6$
pentacene	$C_6C_6C_6C_6C_6$
pentaphene	$C_6C_6C_6C_6C_6$
perylene	$C_6C_6C_6C_6C_6$
picene	$C_6C_6C_6C_6C_6$
pleiadene	$C_7C_6C_6C_6$
tetracene	$C_6C_6C_6C_6$
tetraphene	$C_6C_6C_6C_6$
chrysene	$C_6C_6C_6C_6$
pyrene	$C_6C_6C_6C_6$
triphenylene	$C_6C_6C_6C_6$
aceanthrylene	$C_6C_6C_6C_5$
acephenanthrylene	$C_6C_6C_6C_5$
fluoranthene	$C_6C_6C_6C_5$
anthracene	$C_6C_6C_6$
phenanthrene	$C_6C_6C_6$
phenalene	$C_6C_6C_6$
fluorene	$C_6C_6C_5$
acenaphthylene	$C_6C_6C_5$
biphenylene	$C_6C_6C_4$
s-indacene	$C_6C_5C_5$
as-indacene	$C_6C_5C_5$
heptalene	C_7C_7
azulene	C_7C_5
naphthalene	C_6C_6
indene	C_6C_5
pentalene	C_5C_5

Monocyclic hydrocarbons (annulenes and benzene, in decreasing order of size)

P-26 PHANE NOMENCLATURE

P-26.0 Introduction
P-26.1 Concepts and terminology
P-26.2 Components of phane parent names
P-26.3 Superatom locants and amplificant attachment locants
P-26.4 Numbering of phane parent hydrides
P-26.5 Skeletal replacement (‘a’) nomenclature in phane nomenclature
P-26.6 Other aspects of phane nomenclature

P-26.0 INTRODUCTION

This section is based on the publication ‘Phane nomenclature, Part I. Phane parent names’ (ref. 5) and this new edition contains no modifications or changes to the recommendations contained therein except a change in the usage of brackets for heterocyclic amplificants which require locants.

When a phane system contains a heterocyclic amplificant with locants, they are enclosed in brackets (see P-26.4.2.2, example 1 and P-26.5.1, example 2).

Phane nomenclature is specific to cyclic or acyclic compounds composed of rings or ring systems directly linked to each other or linked by atoms or chains.

Cyclophanes are recognized as a class of compounds (refs. 19, 23). The term originally applied to compounds having two 1,4-phenylene groups held face to face by $-[CH_2]_n-$ bridges (ref. 23). It now designates compounds having:

(a) saturated and/or mancude rings or ring systems, or assemblies of saturated and/or mancude rings or ring systems and;

(b) atoms and/or saturated or unsaturated chains as alternate components of a large ring.

Phane nomenclature is used to name cyclophanes and has been extended to linear compounds (for the use of phane nomenclature in the generation of preferred IUPAC names see P-52.2.5).

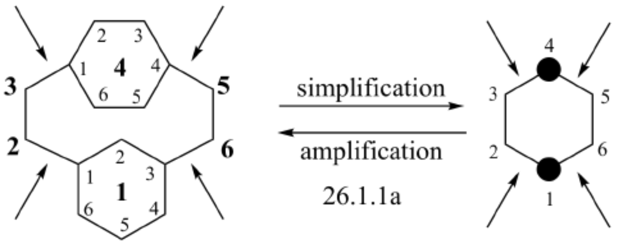
P-26.1 CONCEPTS AND TERMINOLOGY

Definitions of terms that will be encountered in the construction of phane names are given below. These terms refer to types of operations, to the components of phane names, and to details of structures involved in the operations.

P-26.1.1 Simplification and amplification

The fundamental operations of phane nomenclature are illustrated in Fig. 2.1. The operation proceeding from left to right is called simplification; the reverse operation is called amplification, or phane replacement.

The simplification operation illustrates the initial step in the process of constructing a phane name, namely, the replacement of nomenclaturally significant segments of a complex cyclic structure by single atom symbols, called superatoms, thus producing a simplified skeleton that can more easily be named. The phane parent hydride name is then formed from the name of the simplified skeleton and those of the cyclic components (called amplificants) that were simplified to superatoms. In contrast to other bonds associated with the amplificant, the bonds marked by arrows in Fig. 2.1 do not disappear in the simplification or amplification operations.



phane parent skeleton
graph A

simplified skeleton
graph B

Fig. 2.1. Phane nomenclature conversion diagram

P-26.1.2 Simplified skeleton of the phane parent hydride, simplified phane parent graph, simplified skeletal name, and skeletal locants.

Graph B in Fig. 2.1 at which simplication ends and amplification starts is called the simplified skeleton of the phane parent hydride, or simply the simplified skeleton, and is represented by a simplified phane parent graph. Its name is the simplified skeletal name. A simplified skeletal name implies a specific skeletal numbering; its locants are the skeletal locants, which become the primary locants for the phane parent hydride. In Fig. 2.1, the skeletal locants are denoted by large numbers; they are the same in the simplified skeleton and in the phane parent skeleton.

P-26.1.3 Superatom and superatom locants

The 'atoms' of the simplified skeleton shown by the symbol • in positions '1' and '4' in graph B in Fig. 2.1 that appear on simplification and disappear in amplification are called superatoms. Their locants are called superatom locants.

P-26.1.4 Amplificant, amplification prefix, and amplificant locants.

A multiatomic unit (a ring or a ring system) of structure replacing a superatom in the amplification operation is called an amplificant; the six-membered rings in Graph A are amplificants. They are expressed in a phane parent name by amplification prefixes. Each such prefix implies a specific numbering of the amplificant; the respective locants are called amplificant locants and are shown as the smaller numbers in Graph A.

P-26.1.5 Attachment atoms and attachment locants.

The atoms of an amplificant to which the bonds marked by arrows in Fig. 2.1 are attached are called attachment atoms and their locants are attachment locants. In Graph A in Fig. 2.1, amplificant locants ‘1’ and ‘4’ are the attachment locants of the upper ring and amplificant locants ‘1’ and ‘3’ are the attachment locants of the lower ring.

P-26.1.6 Phane parent skeleton, phane parent name, and phane parent hydrides

The skeletal graph at the start of the simplification operation or resulting from an amplification operation is called a phane parent skeleton. Correspondingly, the combination of the simplified skeletal name, amplification prefixes, and the appropriate superatom and attachment locants, is called a phane parent name. The term parent implies that it can be combined with names for other components derived from the operations of systematic nomenclature of organic chemistry, such as substituent prefixes, hydrogenation prefixes and endings, and characteristic group suffixes. In the absence of such other components, the compound is a phane parent hydride, which means that the name implies the order (valence) of all bonds of the skeletal parent and thus the number of hydrogen atoms attached to each of the skeletal atoms.

P-26.2 COMPONENTS OF PHANE PARENT NAMES

P-26.2.1 Simplified skeletal names
P-26.2.2 Amplification prefixes
P-26.2.3 Multiple identical amplificants

P-26.2.1 Simplified skeletal names

A simplified skeletal name consists of the term ‘phane’ preceded by a prefix denoting the structure of the simplified skeleton; this name is a parent for amplification but for no other operation. The simplification operation must be done in such a way that the amplificants can be expressed by amplification prefixes (see P-26.2.2).

A bond order of one is assumed for all bonds expressed by a simplified skeletal name. Atoms not identified by superatoms represent, by convention, carbon atoms with a bonding number (valence) of four in accordance with the principles of nomenclature of organic compounds.

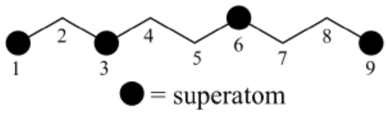
Superatoms of a simplified skeletal name are assigned the lowest locants or the lowest set of locants, consistent with the numbering of the skeletal class to which it belongs. The lowest set of locants is the one that has the locant with the lowest numerical value at the first point of difference, when the sets are compared term by term in order of increasing value (see P-14.3.5).

Four types of simplified skeletal structures are described below, unbranched acyclic (P-26.2.1.1), monocyclic (P-26.2.1.2), polycyclic von Baeyer (P-26.2.1.3), and spiro (P-26.2.1.4).

Names of simplified skeletons consist of, in order, a prefix (‘cyclo’, ‘bicyclo’, ‘spiro’, etc.) indicating the type of structure, a numerical term ‘di’, ‘tri’, ‘tetra’, etc. indicating the number of nodes (including those designating superatoms), and the term phane. No prefix is used to name linear phanes. The nodes are numbered in accordance with the recommended numbering for each type of structure, as indicated in Chapter P-2. Superatoms are given the lowest possible locants.

P-26.2.1.1 Unbranched acyclic simplified skeletal structures

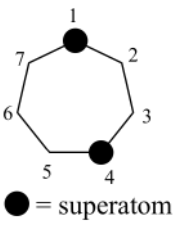
Example:



nonaphane
(see P-26.4.1.2 and the first example of P-26.5.1)

P-26.2.1.2 Monocyclic simplified skeletal structures

Example:

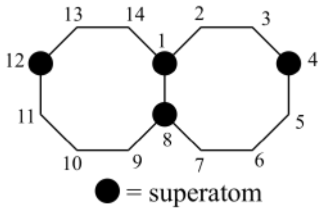


cycloheptaphane
(see the first example of P-26.4.1.4;

the second example of P-26.4.2.2;
and the first example of P-26.4.3.3)

P-26.2.1.3 Polyalicyclic (von Baeyer) simplified skeletal structures

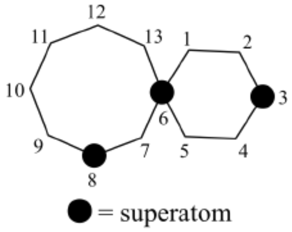
Example:



bicyclo[6.6.0]tetradecaphane
(see the third example of P-26.4.2.2)

P-26.2.1.4 Spiro simplified skeletal structures

Example:



spiro[5.7]tridecaphane
(see the second example of P-26.4.2.4)

P-26.2.2 Amplification prefixes

P-26.2.2.1 Naming amplification prefixes

Names of amplificant prefixes are those of allowed rings or ring systems (see P-26.2.2.2.1) modified by changing the final letter ‘e’ to ‘a’, or adding the letter ‘a’ when no final letter ‘e’ is present.

Examples:

pyrrole (PIN)	pyrrola (preferred prefix)
furan (PIN)	furana (preferred prefix)
pyran (PIN)	pyrana (preferred prefix)
naphthalene (PIN)	naphthalena (preferred prefix)
anthracene (PIN)	anthracena (preferred prefix)

P-26.2.2.2 Parent hydride names for deriving amplification prefixes

P-26.2.2.2.1 Allowed parent hydrides

An amplification prefix can be derived from monocyclic rings and polycyclic ring systems having the maximum number of noncumulative double bonds (mancude), bridged fused ring systems, saturated monocyclic rings, saturated bicycloalkanes and polycycloalkanes (von Baeyer hydrocarbons), and spiro alkanes. In addition stereoparents are allowed, such as ‘gonane’ or ‘morphinan’ (see Chapter P-10). Numbering of the parent is retained.

P-26.2.2.2.2 Disallowed names of parent hydrides

(a) the following parent hydride names are not allowed:

(1) spirobi names such as ‘1,1′-spirobi[indene]’ (PIN);

(2) spiro ring systems with at least one fused ring system or polycycloalkane ring system, such as ‘spiro[[1,3]dioxolane-2,1′-indene]’ (PIN) and ‘spiro[bicyclo[2.2.2]octane-2,1′-cyclohexane]’ (PIN)

(3) ring assembly names, such as ‘1,1′-biphenyl’ (PIN).

(b) modified parent hydride names (the corresponding modifications are made once the phane parent hydride has been fully constructed):

(1) by ’hydro’ prefixes, such as ‘9,10-dihydroanthracene’ (PIN);

(2) by '-ene' or '-yne' endings, such as 'cyclohexene' (PIN);

(3) by skeletal replacement ('a') terms, such as '1-azabicyclo[3.2.1]octane' (PIN);

(4) by suffixes, such as 'cyclohexanecarboxylic acid' (PIN) and 'cyclohexanone' (PIN);

(5) by substitutive prefixes, such as 'ethylbenzene' (PIN).

(c) functional parent structures having retained names, such as 'benzoic acid' (PIN) and 'aniline' (PIN).

(d) names of cyclic compounds formed by functional class nomenclature, such as 'benzyl chloride'.

(e) partially hydrogenated parent hydride names having retained names, such as 'indane' and 'chromane'.

P-26.2.2.3 Order of citation of amplification prefixes

Amplification prefixes are cited in a name in decreasing order of their ring seniority (see P-44.2).

P-26.2.3 Multiple identical amplificants

Amplificants occurring more than once in a parent phane skeleton are expressed by use of an appropriate multiplicative term, either 'di', 'tri', etc. or 'bis', 'tris', etc. It is not necessary that the identical amplification prefixes have also identical locants.

P-26.2.3.1 The multiplying prefixes 'di', 'tri', 'tetra', etc. are used in front of simple amplification prefixes, for example dibenzena, tripyridina.

P-26.2.3.2 The multiplying prefixes 'bis', 'tris', 'tetrakis', etc. are used before an amplification prefix when it begins with a multiplying prefix as in 'bicyclo[2.2.1]heptane' (PIN), '1,3-dioxole' (PIN); or it begins with a name component that could be preceded by a multiplying prefix indicating a multiple occurrence of that name component, as in '1,4-oxazine' (PIN), '2-benzoxepine' (PIN), and '1,4- methanonaphthalene' (PIN).

P-26.3 SUPERATOM LOCANTS AND AMPLIFICANT ATTACHMENT LOCANTS

After the simplified skeletal name and the amplification prefix names have been determined, the phane parent hydride name is completed by adding the locants for the superatoms and the attachment locants. These locants are cited before an amplification prefix; the superatom locant is cited first followed by the attachment locants enclosed in parentheses.

P-26.3.1 Superatom locants

Superatom locants are assigned the lowest locants of the simplified skeleton consistent with the numbering of the class to which it belongs. An amplification prefix preceded by a multiplicative term indicating the presence of like amplificants requires the appropriate number of superatom locants, which are cited in ascending numerical order.

When like amplificants also have identical attachment locants, their attachment locants are arranged in ascending numerical order of the first cited superatom locant.

P-26.3.2 Attachment locants

The locants in parentheses in a phane parent hydride name are the attachment locants of the amplificant whose position in the phane parent skeleton is specified by the preceding superatom locant. The specific order of the attachment locants in the set describes precisely how their respective amplificant is attached to the rest of the phane parent skeleton. Amplificants retain the locants of the cyclic parent hydride from which they are derived.

P-26.3.2.1 Identical attachment locant sets for multiple identical amplificants are cited only once in a name; they follow the set of superatom locants corresponding to the identical amplificants.

Example:

1,4(1,4)-dibenzenacyclohexaphane (PIN)
[not 1(1,4),4(1,4)-dibenzenacyclohexaphane;
see second example of P-26.4.1.4]

P-26.3.2.2 The locants in an attachment locant set are arranged so that of any two locants the one cited first is adjacent to the lower locant of the phane parent skeleton.

Example:

1(1,3),4(1,4)-dibenzenacycloheptaphane (PIN)
[not 1(1,4),4(1,3)-dibenzenacycloheptaphane;
see second example of P-26.4.2.2]

P-26.4 NUMBERING OF PHANE PARENT HYDRIDES

The following rules are used for numbering phane parent hydrides. These rules are hierarchical; that is, each particular rule is applied only to alternatives not eliminated by preceding rules.

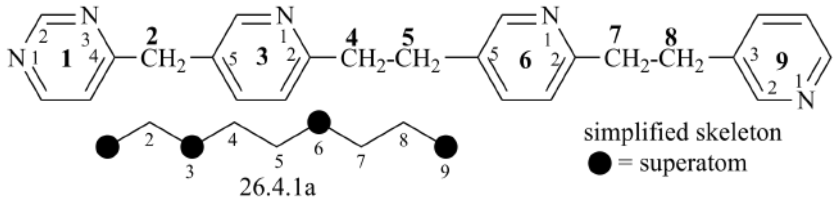
P-26.4.1 Numbering of phane parent skeletons and amplificants

P-26.4.1.1 The numbering of a phane parent skeleton is first determined by the rules governing the appropriate skeletal class to which it belongs. When because of skeletal symmetry, these rules leave alternatives, the numbering that gives the lowest set of locants for the superatoms is selected. The lowest set of locants is the one that has the lowest numerical value at the first point of difference, when the sets are compared term by term in increasing numerical value, as defined in P-14.3.5.

P-26.4.1.2 Numbering of an amplificant is determined primarily by the numbering rules that apply to the parent name from which the amplification prefix is derived. When there is a choice, the general rule of lowest locants is used, as described in the preceding rule.

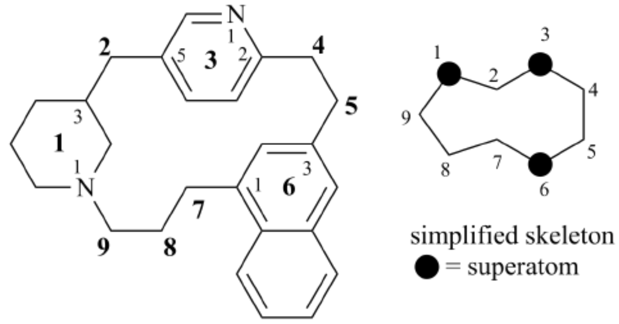
These two rules, P-26.4.1.1 and P-26.4.1.2, are illustrated by the following examples.

Examples:



26.4.1a

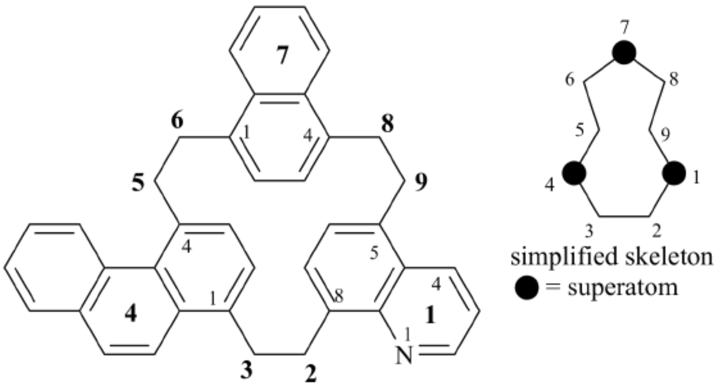
1(4)-pyrimidina-3,6(5,2),9(3)-tripyridinanonaphane (PIN)
[not 9(4)-pyrimidina-1(3),4,7(2,5)-tripyridinanonaphane;
the superatom locant set of the PIN, ‘1,3,6,9’, is lower than ‘1,4,7,9’, see P-26.2.1.1 and P-26.4.1.1]
[not 1(4)-pyrimidina-3,6(2,5),9(3)-tripyridinanonaphane;
the first locant of the pyridine attachment locant set, ‘(2,5)’, is not the locant adjacent to the lower locant of the simplified skeleton, see P-26.3.2.2]
[not 1(4)-pyrimidina-3(5,2),6(5,2),9(3)-tripyridinanonaphane;
the identical attachment locant sets ‘(5,2)’ are not contracted as ‘3,6(5,2)’, see P-26.3.2.1]
[not 1(4)-pyrimidina-3,6(3,6),9(3)-tripyridinanonaphane;
the attachment locant set ‘(5,2)’ of the pyridine amplificant in the PIN, written in the ascending numerical order ‘(2,5)’ for comparison, is lower than the set ‘(3,6)’, see P-26.4.1.2]



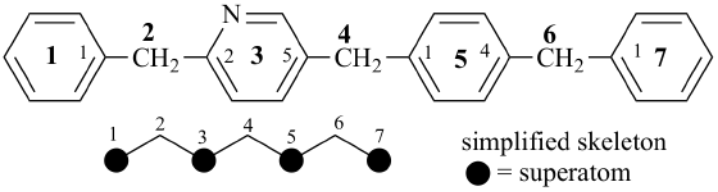
3(5,2)-pyridina-1(3,1)-piperidina-6(3,1)-naphthalenacyclononaphane (PIN)
[not 1(5,2)-pyridina-3(3,1)-piperidina-7(3,1)-naphthalenacyclononaphane
nor 7(5,2)-pyridina-5(1,3)-piperidina-1(3,1)-naphthalenacyclononaphane;
the superatom locant set of the PIN, ‘1,3,6’, is lower than the locant set ‘1,3,7’ or ‘1,5,7’
in either of the other names. see P-26.4.1.1]
[not 3(2,5)-pyridina-1(1,3)-piperidina-6(1,3)-naphthalenacyclononaphane;
the first locant of each the attachment locant sets ‘(2,5)’, ‘(1,3)’, and ‘(1,3)’
for the pyridine, piperidine, and naphthalene amplificants, respectively,
is not the locant adjacent to the lower locant of the simplified parent skeleton, see P-26.3.2.2]

P-26.4.1.3 Amplification of symmetrical simplified phane skeletons with at least two superatoms representing different amplificants results in the loss of symmetry and creates numbering alternatives. In such cases, the lower available superatom locant is assigned to an amplificant that appears earlier in the seniority of rings and ring systems (see P-44.2). The application of this procedure may require a sequence of steps. First, the lowest available superatom locant(s) is (are) assigned to the amplificants appearing first in the seniority order. Then, the same procedure is applied successively to assign remaining superatom locants to the rest of the amplificants.

Example:



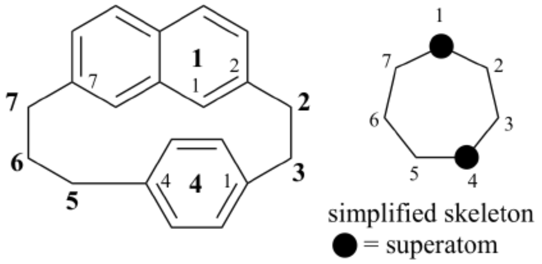
1(8,5)-quinolina-4(1,4)-phenanthrena-7(1,4)-naphthalenacyclononaphane (PIN)
[not 1(8,5)-quinolina-4(1,4)-naphthalena-7(4,1)-phenanthrenacyclononaphane;
the senior amplificant is quinoline (see P-44.2) and must receive the lowest superatom locant '1';
the phenanthrene amplificant is second in seniority (see P-44.2) and therefore must
be given the second lowest superatom locant '4', see P-26.2.2.3]
[not 1(8,5)-quinolina-4(4,1)-phenanthrena-7(1,4)-naphthalenacyclononaphane;
the attachment locants of the phenanthrene amplificant,'(4,1)', are not correctly cited; the first locant of the
attachment locant set is not the locant adjacent to the lower locant of the simplified parent skeleton, '3', see P-26.3.2.2]



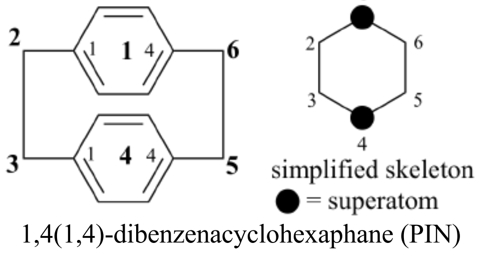
3(2,5)-pyridina-1,7(1),5(1,4)-tribenzenaheptaphane (PIN)
[not 5(5,2)-pyridina-1,7(1),3(1,4)-tribenzenaheptaphane;
the locant '3' for the pyridine amplificant in the PIN is lower than '5', see P-26.3.1]

P-26.4.1.4 When, because of symmetry, these rules leave a choice, an amplificant is numbered in such a way that the lower attachment locant is adjacent to the lower locant of the phane parent skeleton.

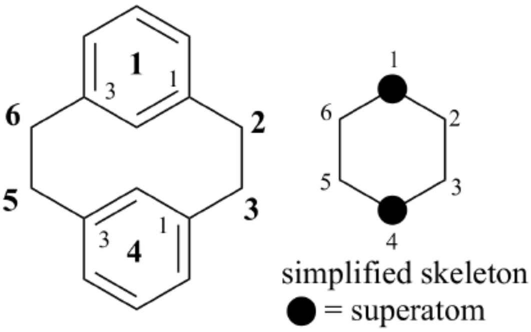
Examples:



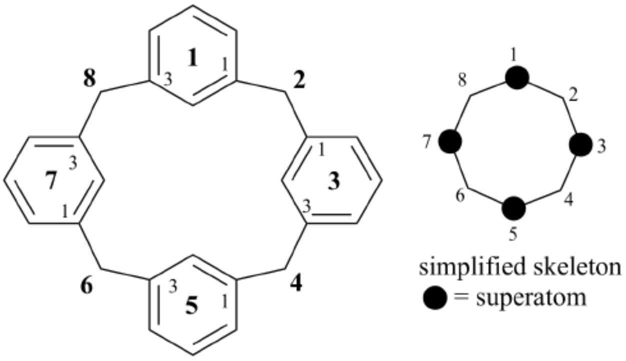
1(2,7)-naphthalena-4(1,4)-benzenacycloheptaphane (PIN)
[the lowest locant set for the superatoms in the phane parent skeleton for the PIN is '1,4';
therefore the senior amplificant, naphthalene (see P-44.2) must be assigned the
superatom locant '1', see P-26.4.1.2 and P-26.4.1.1]
[not 1(2,7)-naphthalena-4(4,1)-benzenacycloheptaphane,
nor 1(7,2)-naphthalena-4(4,1)-benzenacycloheptaphane;
the correct citation for the attachment locant sets, '(1,4)' for benzene and '(2,7)' for the
naphthalene amplificant in the PIN, places the lower attachment locant adjacent to
the lower locant of the simplified parent skeleton (see P-26.3.2.2)]



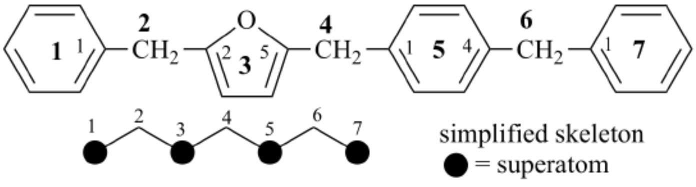
1,4(1,4)-dibenzenacyclohexaphane (PIN)


1
2
3
4
5
6
simplified skeleton
● = superatom

1,4(1,3)-dibenzenacyclohexaphane (PIN)


1
2
3
4
5
6
7
8
simplified skeleton
● = superatom

1,3,5,7(1,3)-tetrabenzenacyclooctaphane (PIN)


1
2
3
4
5
6
7
O
CH2
simplified skeleton
● = superatom

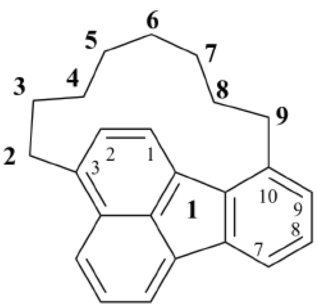
3(2,5)-furana-1,7(1),5(1,4)-tribenzenaheptaphane (PIN)
[not 3(5,2)-furana-1,7(1),5(1,4)-tribenzenaheptaphane;
for superatom **3** the lower attachment locant is not adjacent
to the lower-numbered atom **2** of the simplified skeleton]

P-26.4.2 Numbering of simplified phane skeletons with respect to amplificant numbering.

Numbering alternatives are found in symmetrical simplified skeletons when amplification by a single unsymmetrical amplificant or by identical amplificants having different attachment locants removes the symmetry. Choice among such alternatives is made according to the following rules.

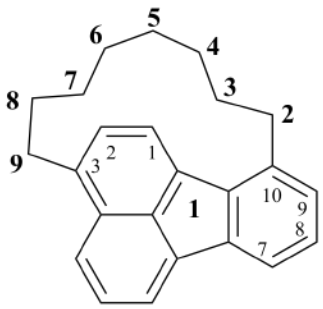
P-26.4.2.1 When a single amplificant is unsymmetrical, the lower locant of the phane parent skeleton must be adjacent to the lower attachment locant of the amplificant.

Example:

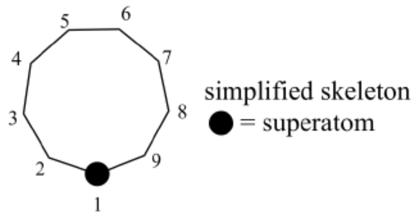

1
2
3
4
5
6
7
8
9
10

(**I**)

not


1
2
3
4
5
6
7
8
9
10

(**II**)

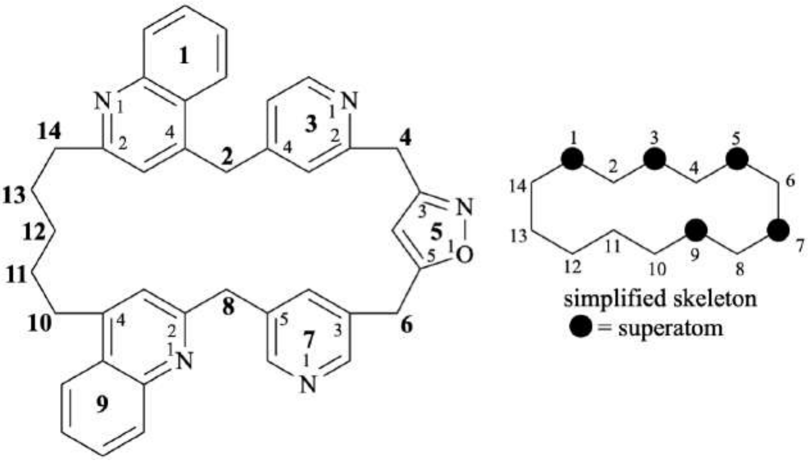

1
2
3
4
5
6
7
8
9
simplified skeleton
● = superatom

1(3,10)-fluoranthenacyclononaphane (**I**)
[not 1(10,3)-fluoranthenacyclononaphane (**II**);

the lower amplificant locant ‘3’ must be adjacent to the lower simplified parent skeletal locant ‘2’]
3,10-octanofluoranthene (PIN) [see P-52.2.5.1 (1)]

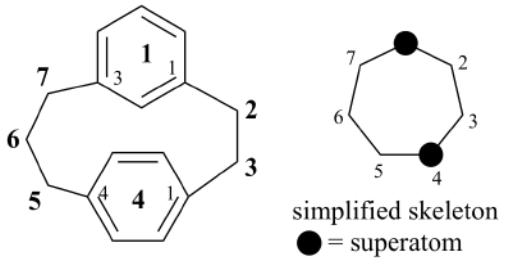
P-26.4.2.2 When two amplificants can be given the lower of two superatom locants, the lower locant is assigned to the superatom representing the amplificant with the lower set of attachment locants. When necessary, this procedure is applied to other amplificants in accordance with their order of seniority until two or more identical amplificants have different attachment locants (see last example).

Examples:

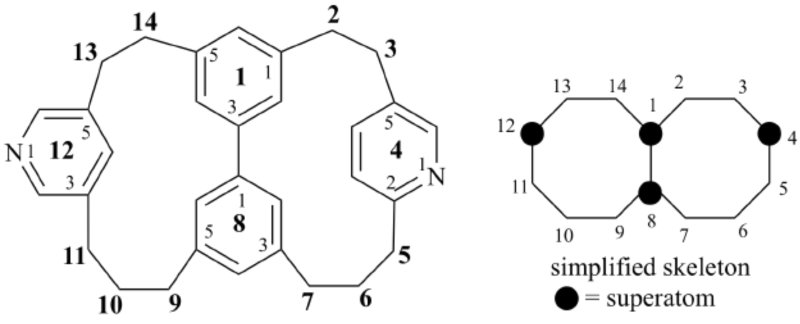

1
N
1
2
4
3
N
1
2
4
2
4
14
13
12
11
10
5
3
N
1
O
5
6
8
7
N
1
3
5
9
N
1
2
4
simplified skeleton
● = superatom

1(4,2),9(2,4)-diquinolina-3(4,2),7(3,5)-dipyridina-5(3,5)-[1,2]oxazolacyclotetradecaphane (PIN)
{not 1(2,4),9(4,2)-diquinolina-3(5,3),7(2,4)-dipyridina-5(3,5)-[1,2]oxazolacyclotetradecaphane;
the attachment locant set for the senior quinoline amplificants; ‘4,2’ and ‘2,4’, respectively,
when compared in ascending numerical order are the same, but
when the attachment locant sets for the pyridine amplificants, ‘(4,2)’ and ‘(5,3)’,
respectively, are compared in ascending numerical order, ‘(2,4)’ and ‘(3,5)’, respectively,
the former is lower and therefore in the PIN the attachment locant set ‘(4,2)’
is associated with the superatom with the lower locant ‘3’ (see P-26.3.2.2)}

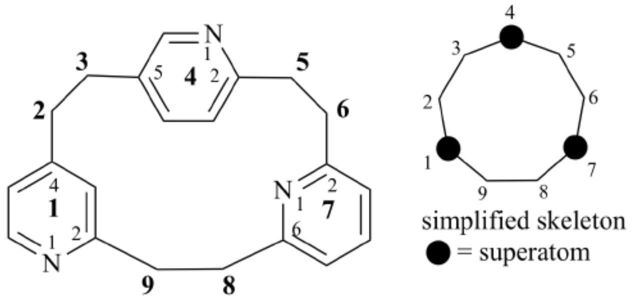
Note: The use of brackets in the name of the third amplificant is a change from PHI-3.2 of ref. 5.


1
3
1
7
2
6
3
5
4
4
1
7
2
6
3
5
4
simplified skeleton
● = superatom

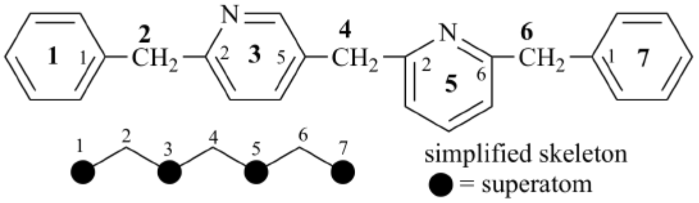
1(1,3),4(1,4)-dibenzenacycloheptaphane (PIN)
[not 1(1,4),4(1,3)-dibenzenacycloheptaphane;
the lower attachment locant set ‘(1,3)’ is not associated with the superatom having the lower locant]
[not 1(1,3),4(4,1)-dibenzenacycloheptaphane;
in the attachment locant set ‘(4,1)’, the first locant is
not the one adjacent to the lower locant of the simplified parent skeleton, see P-26.3.2.2]


14
2
13
3
5
1
1
3
N
1
12
5
3
5
4
1
N
2
1
8
5
3
11
5
10
9
7
6
13
14
2
3
1
12
4
11
5
8
10
9
7
6
simplified skeleton
● = superatom

4(5,2),12(3,5)-dipyridina-1,8(1,3,5)-dibenzenabicyclo[6.6.0]tetradecaphane (PIN)
[not 4(3,5),12(2,5)-dipyridina-1,8(1,3,5)dibenzenabicyclo[6.6.0]tetradecaphane;
for the pyridine amplificants the attachment locant set ‘(5,2)’, when compared in ascending numerical order,
that is, ‘(2,5)’, is lower than ‘(3,5)’; therefore in the PIN, the pyridine amplificant
with the locant set ‘(5,2)’ must be associated with the lower superatom locant, ‘4’]


simplified skeleton
● = superatom

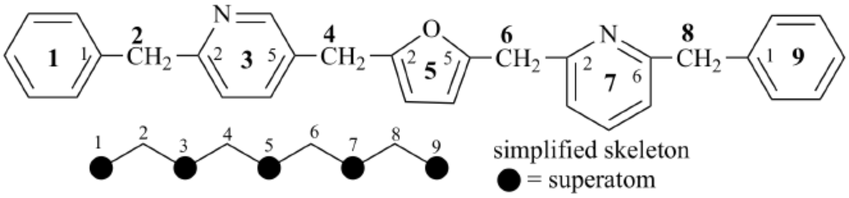
1(4,2), 4(5,2),7(2,6)-tripyridinacyclononaphane (PIN)
[the attachment locant sets '(2,4)', '(2,5)', and '(2,6)' must be assigned to superatoms '1', '4', and '7', respectively; the arrangement of the locants in each set is governed by P-26.3.2.2]


simplified skeleton
● = superatom

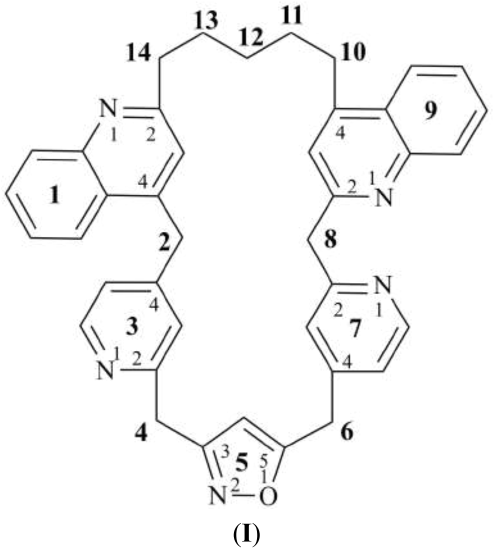
3(2,5),5(2,6)-dipyridina-1,7(1)-dibenzenaheptaphane (PIN)
[not 3(6,2),5(5,2)-dipyridina-1,7(1)-dibenzenaheptaphane;
the attachment locants '2,5' and '2,6' of the pyridine amplificants
must be assigned to superatoms '3' and '5', respectively (see P-26.3.2)]

P-26.4.2.3 If, after the application of P-26.4.2.2, a choice is still necessary and a single unsymmetrical amplificant remains, P-26.4.2.1 is applied to the single unsymmetrical amplificant.

Examples:

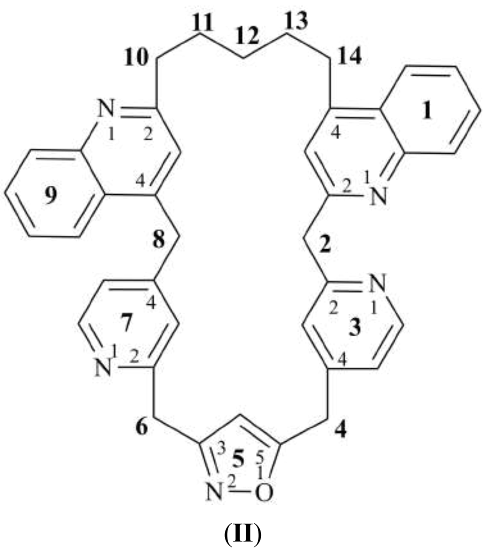

simplified skeleton
● = superatom

3(2,5),7(2,6)-dipyridina-5(2,5)-furana-1,9(1)-dibenzenanonaphane (PIN)
[not 3(2,5),7(2,6)-dipyridina-5(5,2)-furana-1,9(1)-dibenzenanonaphane;
the first locant of the attachment locant set '5,2' is not the locant adjacent
to the lower locant of the simplified parent skeleton, '4' (see P-26.3.2.2)]

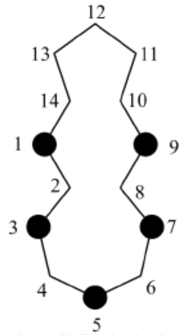


(I)

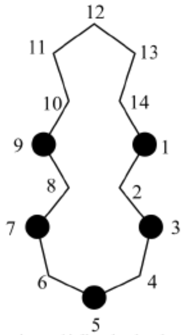
not



(II)


12
13
11
14
10
1
9
2
8
3
7
4
6
5

simplified skeleton
● = superatom
(**I**)

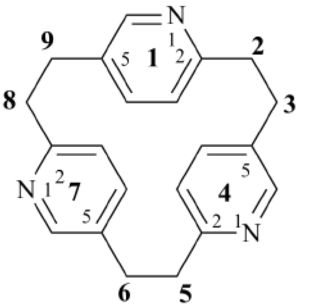

12
11
13
10
14
9
1
8
2
7
3
6
4
5

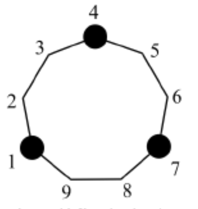
simplified skeleton
● = superatom
(**II**)

1(4,2),9(2,4)-diquinolina-3,7(4,2)-dipyridina-5(3,5)-[1,2]oxazolacyclotetradecaphane (**I**) (PIN)
[not 1(2,4),9(4,2)-diquinolina-3,7(2,4)-dipyridina-5(5,3)-[1,2]oxazolacyclotetradecaphane (**II**);
each of the identical pairs of amplificants, quinolina and pyridina,
have identical attachment locants, '(2,4)' and '(2,4)', respectively;
the single unsymmetrical amplificant, 1,2-oxazola, remains to which P-26.4.2.1 applies;
its lower attachment locant '3' must be adjacent to the
lower locant of the simplified parent skeleton, '4']

P-26.4.2.4 When two numberings for a simplified phane skeleton are still possible, the selected numbering is that which gives the lower locant set when attachment locants of all amplificants, as they appear in the name, are compared in the increasing order of their corresponding superatom locants.

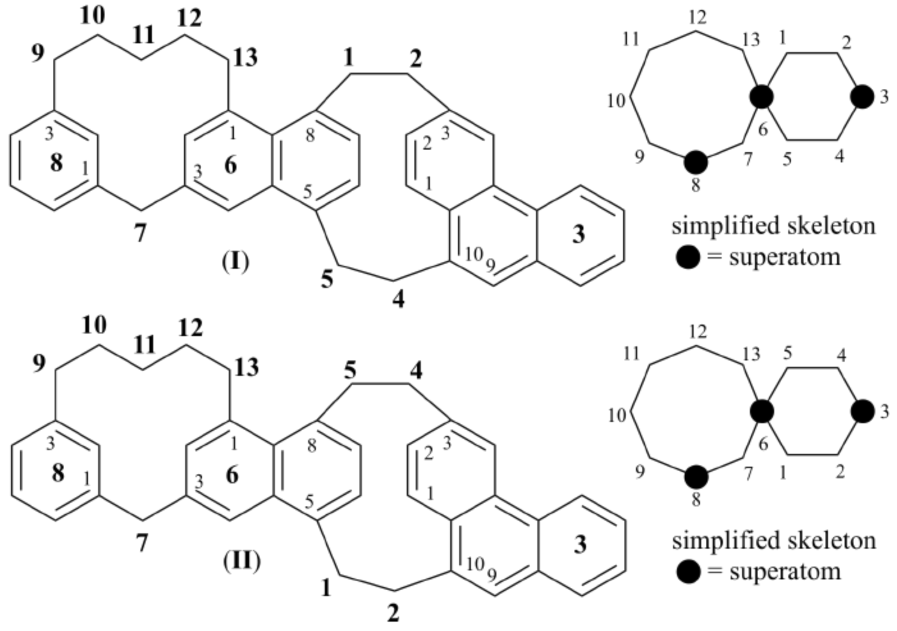
Examples:


N
1
9
5
1
2
2
8
3
2
N
1
7
5
5
4
2
1
N
6
5

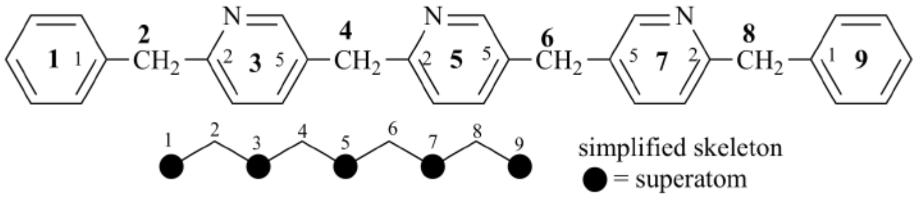


simplified skeleton
● = superatom

1(2,5),4,7(5,2)-tripyridinacyclononaphane (PIN)
[not 1(5,2),4,7(2,5)-tripyridinacyclononaphane;
when compared in the order of increasing value of the corresponding superatoms,
the amplificant locant set '(2,5)(5,2)(5,2)' in the PIN is lower than '(5,2)(2,5)(2,5)']


10
11
12
9
13
1
2
3
8
1
1
8
3
6
2
3
1
5
10
9
3
7
(I)
5
4
12
11
13
1
2
10
3
6
9
7
5
4
8
simplified skeleton
● = superatom
10
11
12
9
13
5
4
3
8
1
1
8
3
6
2
3
1
5
10
9
3
7
(II)
1
2
12
11
13
5
4
10
3
6
9
7
1
2
8
simplified skeleton
● = superatom

3(3,10)-phenanthrena-6(8,5,3,1)-naphthalena-8(1,3)-benzenaspiro[5.7]tridecaphane (**I**) (PIN)
[not 3(10,3)-phenanthrena-6(5,8,3,1)-naphthalena-8(1,3)-benzenaspiro[5.7]tridecaphane (**II**);
the set of attachment locants '(3,10)(8,5,3,1)(1,3)' in the PIN cited for comparison
in the order of the increasing value of their corresponding superatom locants,
is lower than the corresponding set of attachment locants, '(10,3)(5,8,3,1)(1,3)']



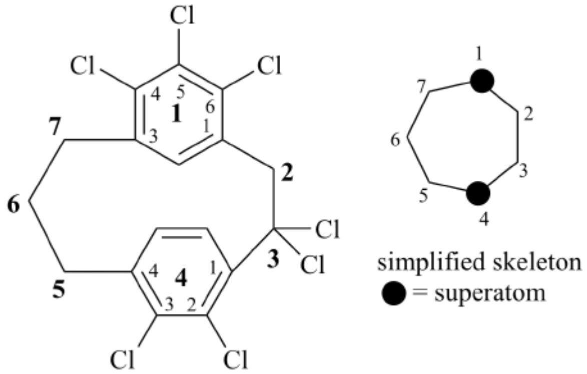
3,5(2,5),7(5,2)-tripyridina-1,9(1)-dibenzenanonaphane (PIN)
[not 3(2,5),5,7(5,2)-tripyridina-1,9(1)-dibenzenanonaphane;
the attachment locants set '(2,5)(2,5)(5,2)' in the PIN, compared
in the order of the increasing value of their corresponding superatom locants,
is lower than the corresponding set of attachment locants,'(2,5)(5,2)(5,2)']

P-26.4.3 Numbering of phane parent hydrides

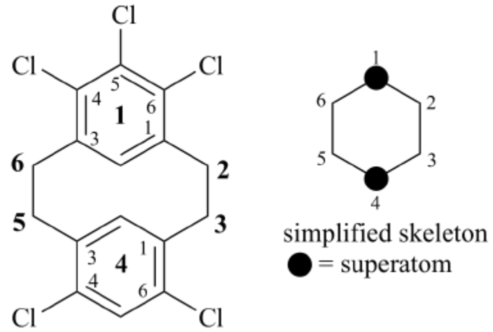
P-26.4.3.1 In a phane parent hydride, the locants for atoms that do not belong to amplificants are the locants of the simplified skeleton. However, locants for the atoms of the amplificants must be distinguished from the arabic number locants of the simplified skeleton. Thus, locants for amplificant atoms are constructed by citing the actual locants of the amplificant as superscripts to the locant of the superatom that represents the amplificant in the simplified skeleton.

P-26.4.3.2 In a substituted phane parent hydride name, a series of composite locants based on the superatom locant must not be contracted. As is the rule for citing locants in front of detachable prefixes, there must be a number of locants corresponding to the multiplying prefix, 'di', 'tri', etc. in front of the prefix.

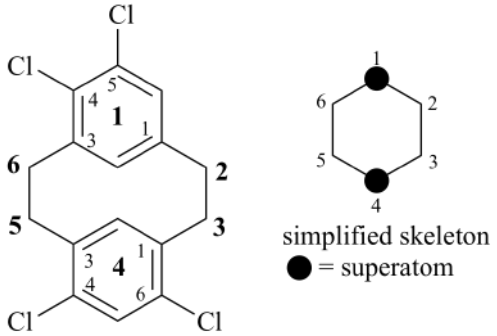
P-26.4.3.3 The seniority of a composite locant is determined first on the basis of its primary locants, i.e., the locants of the phane parent skeleton, and, if these locants are identical, on the basis of the complete composite locant itself, i.e., the primary locant and its superscripts.



1^{4},1^{5},1^{6},3,3,4^{2},4^{3}-heptachloro-1(1,3),4(1,4)-dibenzenacycloheptaphane (PIN)
[not $1^{4,5,6}$,3,3,$4^{2,3}$-heptachloro-1(1,3),4(1,4)-dibenzenacycloheptaphane;
superscript locants denoting positions on amplificants are not contracted (see P-26.4.3.2)]
[not 1^{2},1^{3},2,2,4^{4},4^{5},4^{6}-heptachloro-1(1,4),4(1,3)-dibenzenacycloheptaphane;
the amplificant with the lower attachment locant set
is not assigned to the superatom with the lowest locant (see P-26.4.2.2)]



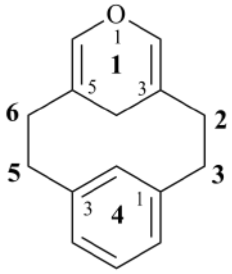
1^{4},1^{5},1^{6},4^{4},4^{6}-pentachloro-1,4(1,3)-dibenzenacyclohexaphane (PIN)
[not 1^{4},1^{6},4^{4},4^{5},4^{6}-pentachloro-1,4(1,3)-dibenzenacyclohexaphane;
the primary locant set '1,1,1,4,4' is lower than the locant set '1,1,4,4,4']



$1^4,1^5,4^4,4^6$-tetrachloro-1,4(1,3)-dibenzenacyclohexaphane (PIN)
[not $1^4,1^6,4^4,4^5$-tetrachloro-1,4(1,3)-dibenzenacyclohexaphane;
the primary locant sets ‘1,1,4,4’ are identical
but the composite locant set in the PIN, ‘$1^4,1^5,4^4,4^6$’, is lower than ‘$1^4,1^6,4^4,4^5$’]

P-26.4.3.4 Indicated hydrogen, when present in amplificants, is placed before the phane parent hydride name and preceded by the appropriate composite locant(s).

Example:



1^4H-1(3,5)-pyrana-4(1,3)-benzenacyclohexaphane (PIN)

P-26.5 SKELETAL REPLACEMENT (‘a’) NOMENCLATURE IN PHANE NOMENCLATURE

Skeletal replacement (‘a’) nomenclature is applied in two ways in phane nomenclature:

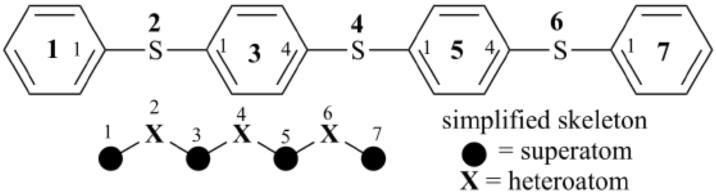
(1) to name phane parent hydrides having heteroatoms located in the simplified parent skeleton, i.e., heteroatoms not in names of amplification prefixes;

(2) to indicate heteroatoms in heterocyclic amplificants whose names cannot be used as amplification prefixes because they, themselves, are named by skeletal replacement (‘a’) nomenclature, for example, heteromonocycles having more than ten members and polycyclic von Baeyer systems.

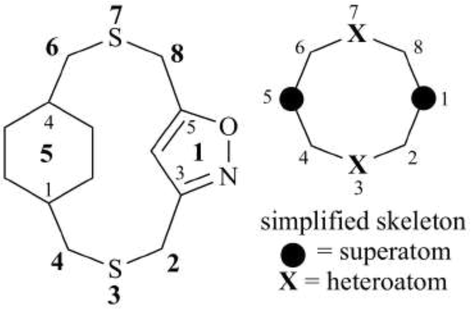
The general principles, conventions, and rules described for skeletal replacement (‘a’) nomenclature in Section P-15.4 are fully applicable to the appropriate phane parent hydrides.

P-26.5.1 Skeletal replacement (‘a’) nomenclature in simplified phane names is accomplished in two steps. First, the parent phane hydrocarbon is named and then the heteroatoms are denoted by means of nondetachable ‘a’ prefixes cited in front of the name so created. Locants for the heteroatoms are assigned according to the numbering of the simplified parent skeleton.

Examples:

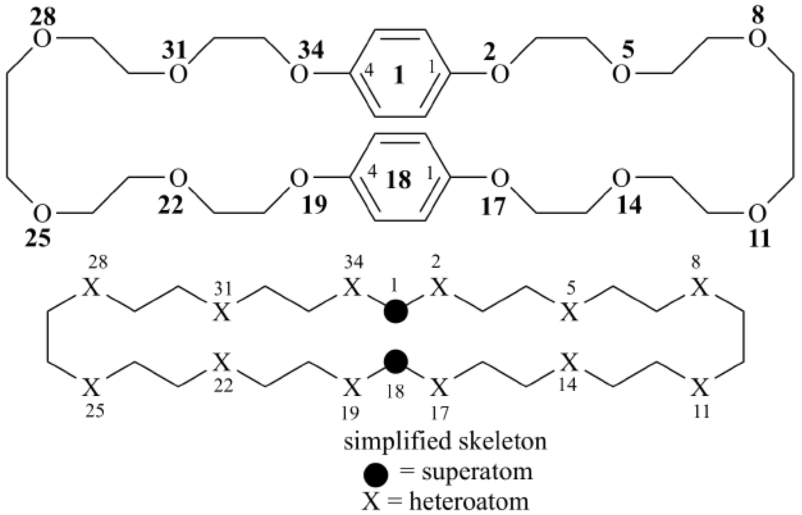


Step 1: 1,7(1),3,5(1,4)-tetrabenzenaheptaphane
Step 2: 2,4,6-trithia-1,7(1),3,5(1,4)-tetrabenzenaheptaphane (PIN)


7
S
6
8
4
5
1
O
N
1
5
3
4
S
2
3
7
X
6
8
5
1
4
X
2
3
simplified skeleton
● = superatom
X = heteroatom

Step 1: 1(3,5)-[1,2]oxazola-5(1,4)-cyclohexanacyclooctaphane
Step 2: 3,7-dithia-1(3,5)-[1,2]oxazola-5(1,4)-cyclohexanacyclooctaphane (PIN)

Note: The use of brackets in the name of the first amplificant is a change from PHI-4.2 of ref. 5.

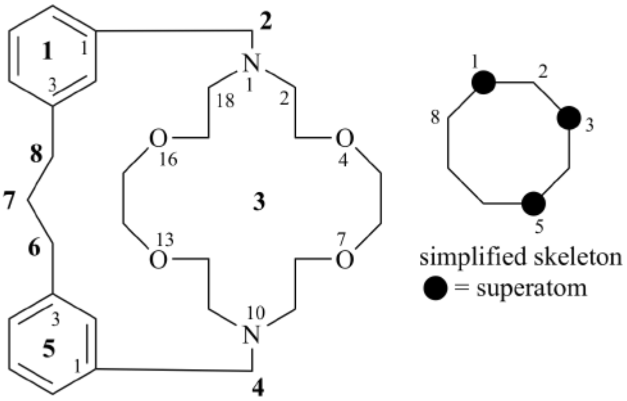

28
31
34
1
2
5
8
25
22
19
18
17
14
11
simplified skeleton
● = superatom
X = heteroatom

Step 1: 1,18(1,4)-dibenzenacyclotetratriacontaphane
Step 2: 2,5,8,11,14,17,19,22,25,28,31,34-dodecaoxa-1,18(1,4)-dibenzenacyclotetratriacontaphane (PIN)

P-26.5.2 Skeletal replacement ('a') nomenclature in amplificants

Locants for heteroatoms in amplificants are assigned according to the numbering of the simplified skeleton and the position of heteroatoms in the amplificants following the instructions in P-26.4 for substituent locants. Thus, positions of heteroatoms in amplificants are described by composite locants.

Example:


1
2
N
3
8
7
6
O
O
O
O
N
5
4
simplified skeleton
● = superatom

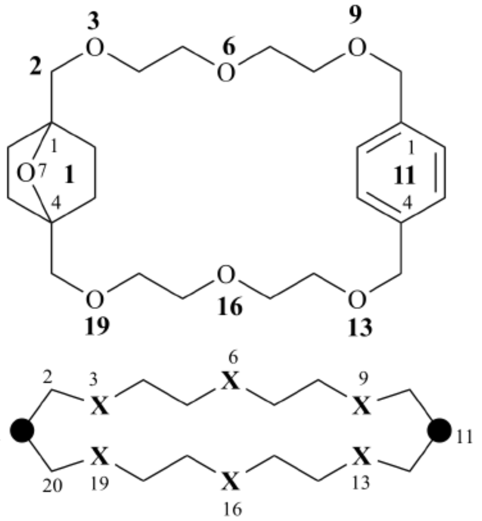
step 1: 3(1,10)-cyclooctadecana-1,5(1,3)-dibenzenacyclooctaphane
3^4,3^7,3^{13},3^{16}-tetraoxa-3^1,3^{10}-diaza-3(1,10)-cyclooctadecana-1,5(1,3)-dibenzenacyclooctaphane (PIN)

Note: Since the numbering of the heteroamplificant is fixed by the locants of the corresponding hydrocarbon amplificant, the numbering of the heteroatoms may not correspond to the numbering of the heteromonocycle itself.

P-26.5.3 Simultaneous skeletal replacement ('a') in simplified skeletal names and amplificants

When skeletal replacement occurs in both simplified skeletons and in amplificants both P-26.5.1 and P-26.5.2 are applied.

Example:



simplified skeleton
● = superatom
X = heteroatom

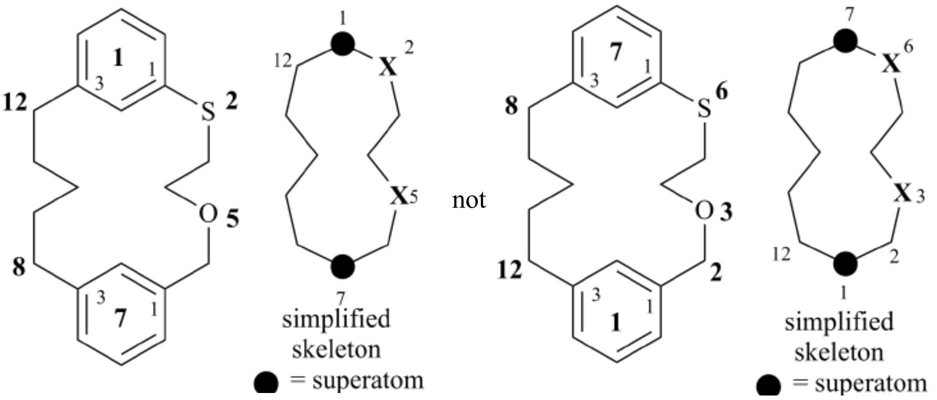
Step 1: 1(1,4)-bicyclo[2.2.1]heptana-11(1,4)-benzenacycloicosaphane
Step 2: 1^7,3,6,9,13,16,19-heptaoxa-1(1,4)-bicyclo[2.2.1]heptana-11(1,4)-benzenacycloicosaphane (PIN)

P-26.5.4 Numbering of heterophane parent hydrides with respect to heteroatoms

When there is a choice for numbering heterocyclic amplificants named by skeletal replacement ('a') nomenclature or for numbering simplified phane skeletons in which skeletal replacement has taken place, the following criteria are applied, in the order given, until a decision is reached.

P-26.5.4.1 Lowest locants are assigned to heteroatoms considered without regard to the nature of the heteroatom, first for the set of primary locants for the heteroatoms, i.e., the locants of the simplified skeleton (without including any superscript numbers), and then, if these locants are identical, with regard to the set of the complete heteroatom locants, which include the primary and the superscript numbers.

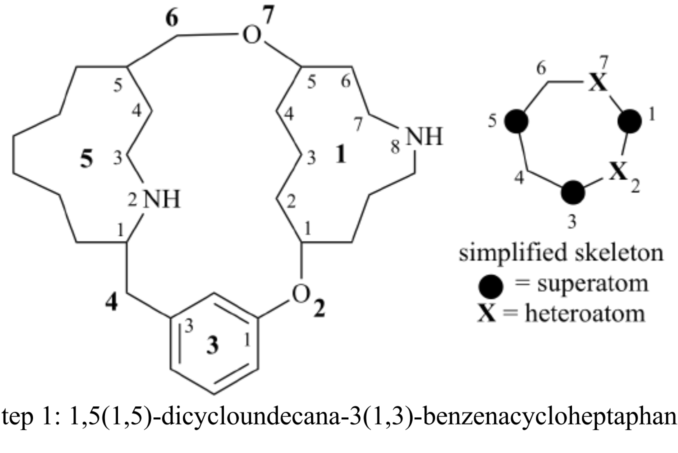
Examples:



simplified skeleton
● = superatom

simplified skeleton
● = superatom

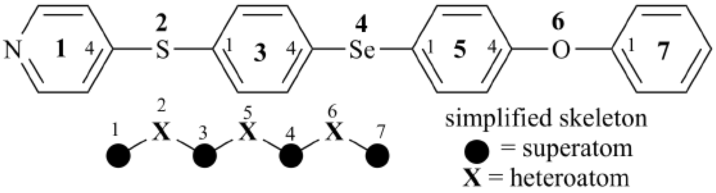
Step 1 : 1,7(1,3)-dibenzenacyclododecaphane [(**I**) and (**II**)]
Step 2: 5-oxa-2-thia-1,7(1,3)-dibenzenacyclododecaphane (**I**) (PIN)
[not 3-oxa-6-thia-1,7(1,3)-dibenzenacyclododecaphane (**II**);
the locant set of the heteroatoms in (**I**) , '2,5',
is lower than the locant set in (**II**), '3,6']



simplified skeleton
● = superatom
X = heteroatom

Step 1: 1,5(1,5)-dicycloundecana-3(1,3)-benzenacycloheptaphane

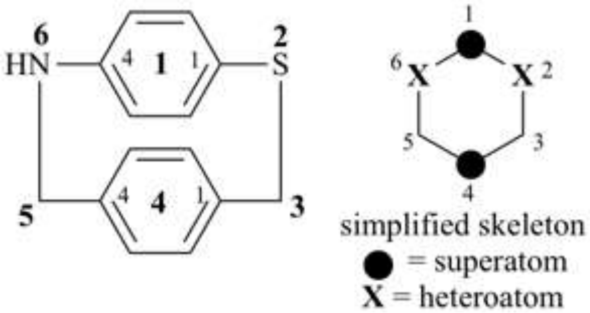
Step 2: 2,7-dioxa-1^{8},5^{2}-diaza-1,5(1,5)-dicycloundecana-3(1,3)-benzenacycloheptaphane (PIN)
[not 4,6-dioxa-1^{2},5^{8}-diaza-1,5(1,5)-dicycloundecana-3(1,3)-benzenacycloheptaphane;
the primary locant set for the heteroatoms in the PIN, cited for comparison
in ascending order ‘1,2,5,7’, is lower than the locant set ‘1,4,5,6’]


N
1
4
2
S
1
3
4
4
Se
1
5
4
6
O
1
7
1
2
X
3
5
X
4
6
X
7
simplified skeleton
● = superatom
X = heteroatom

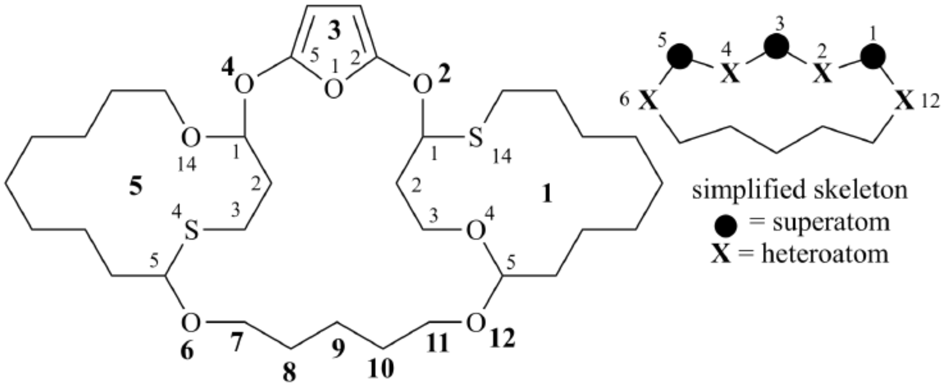
6-oxa-2-thia-4-selena-1(4)-pyridina-3,5(1,4),7(1)-tribenzenaheptaphane (PIN)
[not 2-oxa-6-thia-4-selena-7(4)-pyridina-1(1),3,5(1,4)-tribenzenaheptaphane;
the senior amplificant ‘pyridina’ must receive the lowest possible locant]

P-26.5.4.2 Lowest locants are assigned to heteroatoms considered in the order of their seniority: O > S > Se > Te > N > P > As > Sb > Bi > Si > Ge > Sn > Pb > B > Al > Ga > In > Tl (see P-15.4), first with regard to the set for primary locants for heteroatoms, i.e., the locants of the simplified skeleton (the locants without including any superscript numbers), and then, if these locants are identical, to the set of the complete heteroatom locants, which includes the primary locants and the superscript numbers (see P-26.4.3.3).

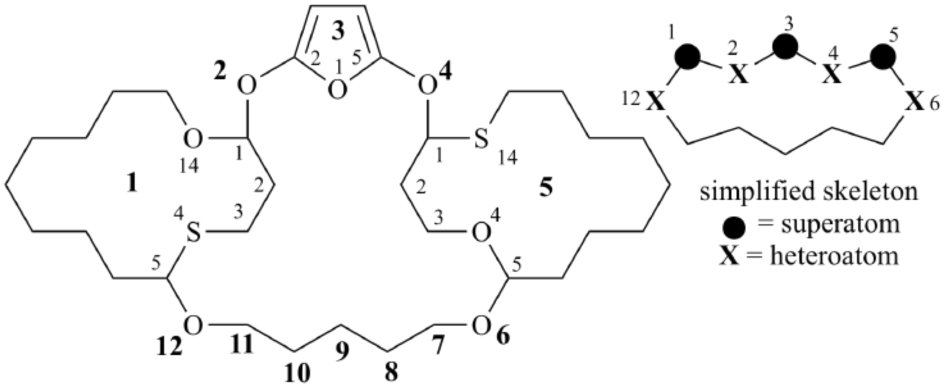
Examples:


6
HN
4
1
1
2
S
4
4
1
5
3
1
6 X
X 2
5
3
4
simplified skeleton
● = superatom
X = heteroatom

Step 1: 1,4(1,4)-dibenzenacyclohexaphane
Step 2: 2-thia-6-aza-1,4(1,4)-dibenzenacyclohexaphane (PIN)
[not 6-thia-2-aza-1,4(1,4)-dibenzenacyclohexaphane;
since the replacement (‘a’) prefix ‘thia’ is senior to ‘aza’ in skeletal replacement (‘a’) nomenclature (see P-15.4), it must be given the lower locant]


3
5
2
1
O
4 O
O 2
O
14
1
2
5
4 S
3
5
O
6
7
8
9
10
11
O 12
S
1
14
2
1
3
O 4
5
5
4
3
2
1
6 X
X
X
X 12
simplified skeleton
● = superatom
X = heteroatom

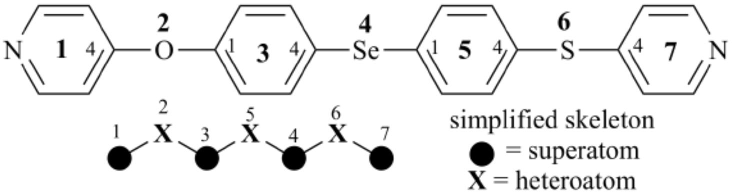
(**I**)


3
2
1
5
2 O
O
O 4
O
14
1
1
2
4 S
3
5
12 O
11
10
9
8
7
O 6
S
1
14
5
2
3
O 4
5
1
2
3
4
5
12 X
X
X
X 6
simplified skeleton
● = superatom
X = heteroatom

(**II**)

Step 1: 3(2,5)-furana-1,5(1,5)-dicyclotetradecanacyclododecaphane
Step 2: 1^{4},2,4,5^{14},6,12-hexaoxa-1^{14},5^{4}-dithia-3(2,5)-furana-1,5(1,5)-dicyclotetradecanacyclododecaphane (**I**) (PIN)

[not 1^{14},2,4,5^{4},6,12-hexaoxa-1^{4},5^{14}-dithia-3(2,5)-furana-1,5(1,5)-dicyclotetradecanacyclododecaphane (**II**); application of P-26.5.4.1 reveals that both the primary locant sets and the primary locant sets including the composite locants for the heteroatoms without regard to the kind of heteroatom are the same for both names, namely, '1,1,2,4,5,5,6,12' and '1^{4},1^{14},2,4,5^{4},5^{14},6,12', respectively. The primary locant sets for the senior prefix 'oxa' are also the same in both cases, '1,2,4,5,6,12', but for the locant sets including composite locants, the locant set for the prefix 'oxa' in (**I**), the PIN, namely, '1^{4},2,4,5^{14},6,12', is lower than the locant set, '1^{14},2,4,5^{4},6,12', for oxa in (**II**)]



2-oxa-6-thia-4-selena-1,7(4)-dipyridina-3,5(1,4)-dibenzenaheptaphane (PIN)
[not 6-oxa-2-thia-4-selena-1,7(4)-dipyridina-3,5(1,4)-dibenzenaheptaphane; the senior replacement ('a') prefix 'oxa' must receive the lowest locant]

P-26.6 OTHER ASPECTS OF PHANE NOMENCLATURE

Part II of phane nomenclature, ref. 6, discusses (1) phane parent hydrides substituted by characteristic groups cited as suffixes. Examples are given in P-62.2.5.3 for amines, in P-63.1.2 for hydroxy compounds, and in P-64.2.2.3 for ketones; and (2) the modification of the degree of hydrogenation; a topic more fully developed in Sections P-31.1.6 and P-31.2.3.3.4.

P-27 FULLERENES

P-27.0 INTRODUCTION

This section is based on the publication 'Nomenclature for the C_{60}-I_{h} and C_{70}-$D_{5h(6)}$ Fullerenes' (ref. 10) and the new edition 2013 contains no modifications or changes to the recommendations therein.

A preliminary survey of the nomenclature and terminology of fullerenes was published in 1997 (ref. 25). This Section is based on the IUPAC Recommendations 2002 (refs. 10, 11), that deal in depth with two fullerenes, i.e. the most commonly known fullerene having 60 carbon atoms and one of its C_{70} homologues.

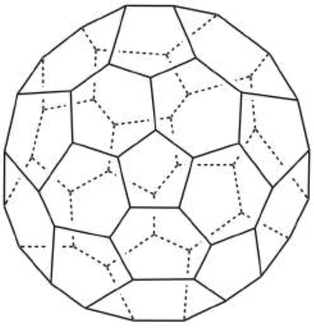
This Section is devoted to parent hydrides only (ref. 10). Derivatives are described in Chapter P-6, radicals and ions are discussed in Chapter P-7. Chapter P-9 includes a brief mention of fullerenes in the discussion on the configurational notation.

P-27.1 Definitions
P-27.2 Fullerene names
P-27.3 Numbering of fullerenes
P-27.4 Structurally modified fullerenes
P-27.5 Replacement of skeletal atoms
P-27.6 Addition of rings and ring systems to fullerenes
P-27.7 Other aspects of fullerene nomenclature

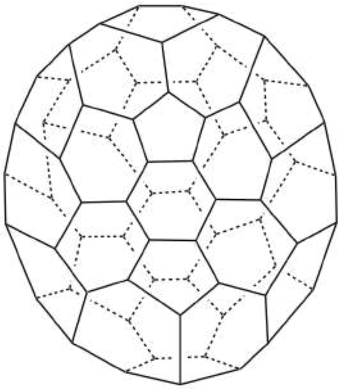
P-27.1 DEFINITIONS

P-27.1.1 Fullerenes

Fullerenes are compounds composed solely of an even number of carbon atoms, which form a cage-like fused-ring polycyclic system with twelve five-membered rings and the rest six-membered rings (see ref. 10). The archetypal example is [60]fullerene, where the atoms and bonds delineate a truncated icosahedron. The term has been broadened to include any closed cage structure consisting entirely of three-coordinate carbon atoms.



C_{60}-I_{h})[5,6]fullerene (PIN)



(C_{70}-$D_{5h(6)}$)[5,6]fullerene (PIN)

P-27.1.2 Fulleranes

Fulleranes are fully saturated fullerenes, for example, $C_{60}H_{60}$.

P-27.1.3 Fulleroids

Heterofullerenes, norfullerenes, homofullerenes, and secofullerenes have been called 'fulleroids' (fullerene-like), because they resemble fullerenes in structure but do not conform to the definition of a fullerene as given above. It is convenient to refer to them as fulleroids and name them as modified fullerenes.

P-27.2 FULLERENE NAMES

P-27.2.1 Systematic names

The recommended systematic names for fullerenes include the number of carbon atoms, the point group symbol, the size of the rings, the relative arrangement of rings, and the term 'fullerene', all combined to give names, such as (C_{60}-I_h)[5,6]fullerene (PIN) and (C_{70}-$D_{5h(6)}$)[5,6]fullerene (PIN) for the two fullerenes discussed in this Section. The parenthetical prefix gives the carbon content and the point group symbol and the bracketed numbers indicate the ring sizes in the fullerene. The latter is important in fullerenes with rings other than five- and six-membered. The subscript (6) following the point group symbol D_{5h} in the latter name indicates that the five-membered ring on the five-fold symmetry axis is surrounded by six-membered rings. This differentiates this fullerene from an isomeric fullerene which has five-membered rings surrounding the five-membered ring on the five-fold symmetry axis, which would have the name (C_{70}-$D_{5h(5)}$)[5,6]fullerene (PIN).

The recommended names have the same information as the corresponding names used by the Chemical Abstracts Service (CAS), but in a different format. The corresponding CAS names are [5,6]fullerene-C_{60}-I_h and [5,6]fullerene-C_{70}-$D_{5h(6)}$, respectively (see ref. 10).

P-27.2.2 Trivial names

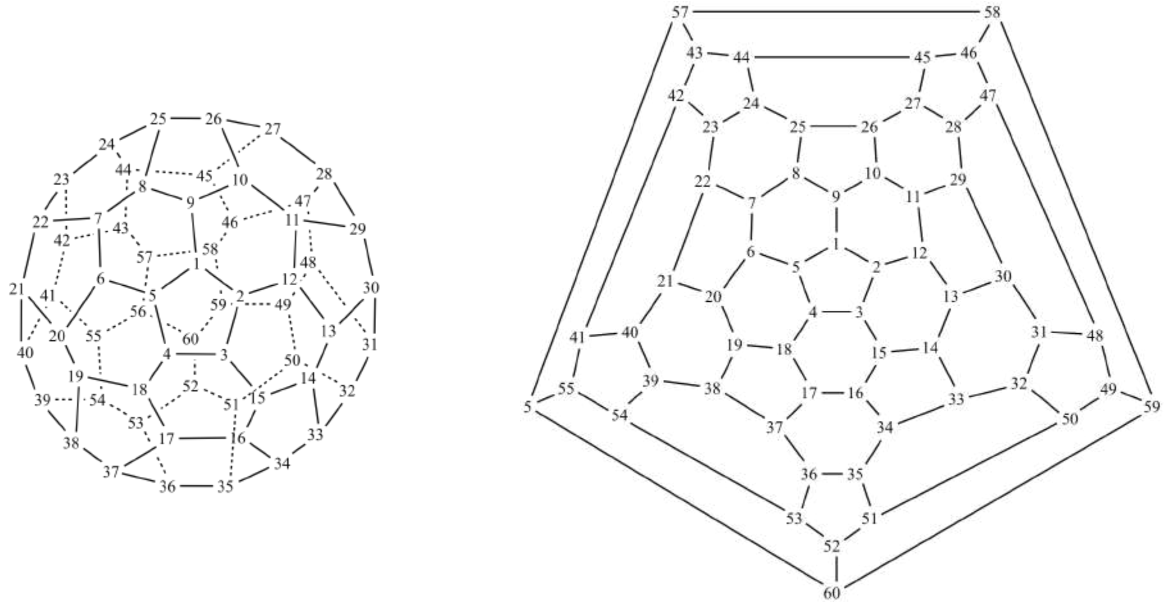
The names [60-I_h]fullerene and [70-D_h]fullerene (shortened to [60]fullerene and [70]fullerene in usage) given in the IUPAC Preliminary Survey (ref. 25) are names first introduced in the literature for the (C_{60}-I_h)[5,6]... and (C_{70}-$D_{5h(6)}$)[5,6]... fullerenes. They were based on a limited definition of fullerenes restricted to five- and six-membered rings. Since important information is missing from these names, they are considered as trivial names only for these specific compounds.

P-27.2.3 Preferred IUPAC names

IUPAC systematic names are preferred to CAS and trivial names. These names are not fully interchangeable. They each depend on a specific methodology for generating names of derivatives. But, most importantly, they do correspond to different numbering systems, one for IUPAC systematic and CAS names, another one for trivial names (see P-27.3). Preferred names for fullerenes and fullerene derivatives are those that use preferred components when a choice is possible (see P-52.2.6).

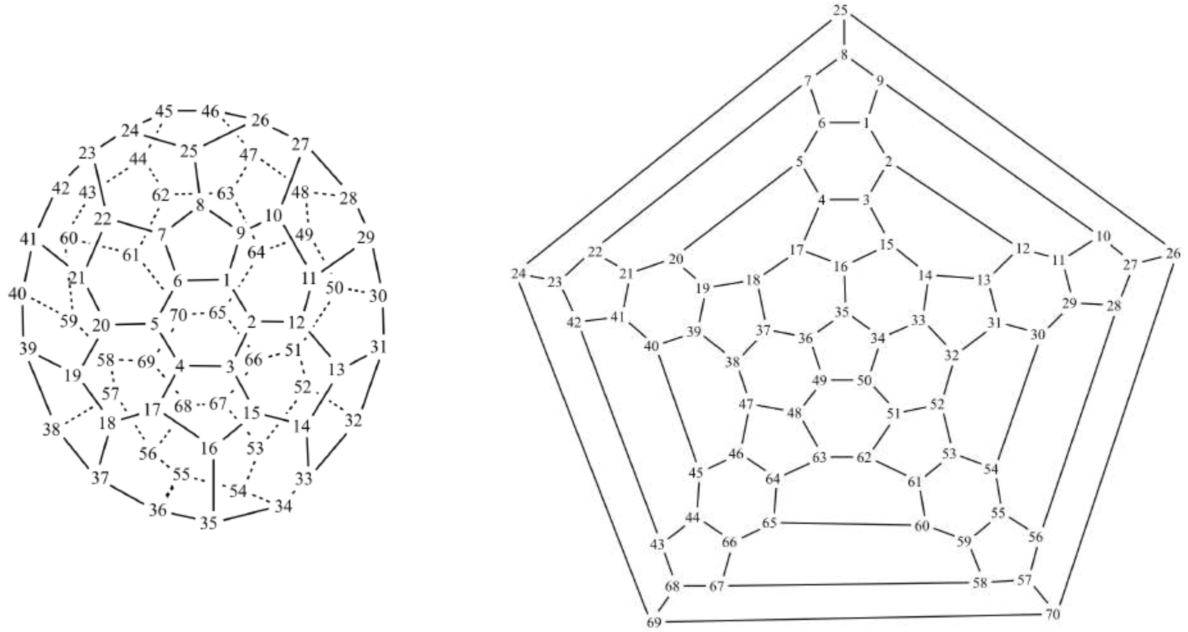
P-27.3 NUMBERING OF FULLERENES

Systematic numbering is not yet a fully solved issue in the nomenclature of fullerenes. The objectives are to achieve a continuous numbering and use a well defined starting point for all fullerenes. The criteria for numbering the (C_{60}-I_h)[5,6]fullerene (PIN) and (C_{70}-$D_{5h(6)}$)[5,6]fullerene (PIN) are discussed in the IUPAC publication (ref. 10). It is important to note that the systematic numbering used with IUPAC systematic names is derived from the system developed by the Chemical Abstracts Service and that the two systems are identical for these two specific fullerenes. The numbering associated with a trivial name may be different if it is based on principles such as 'most reactive bond'. The two systems of numbering are shown below for three-dimensional structures and Schlegel representations.



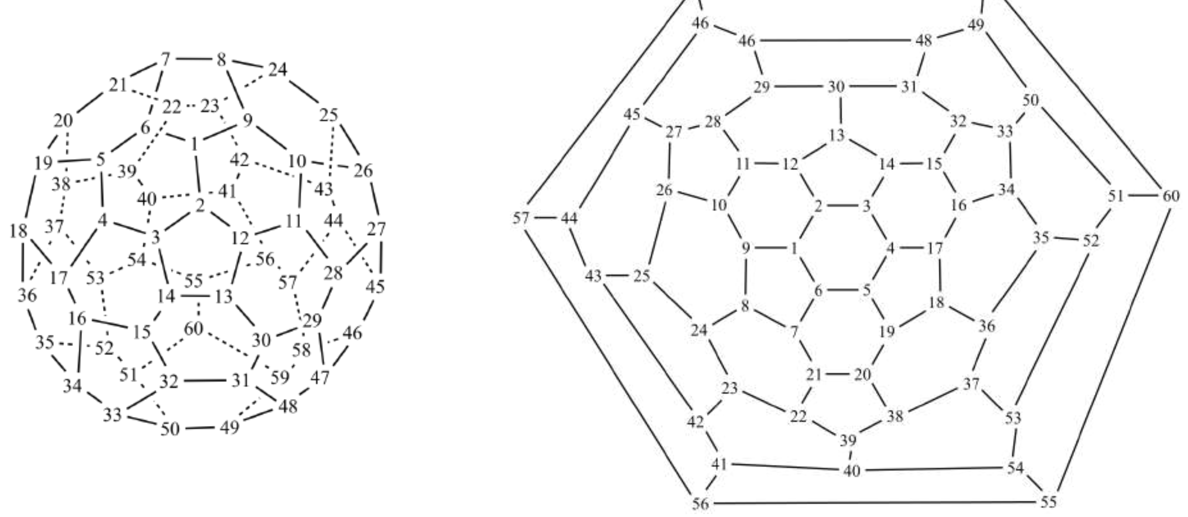
3-D Representation Schlegel representation

(C_{60}-I_h)[5,6]fullerene (PIN; systematic numbering)



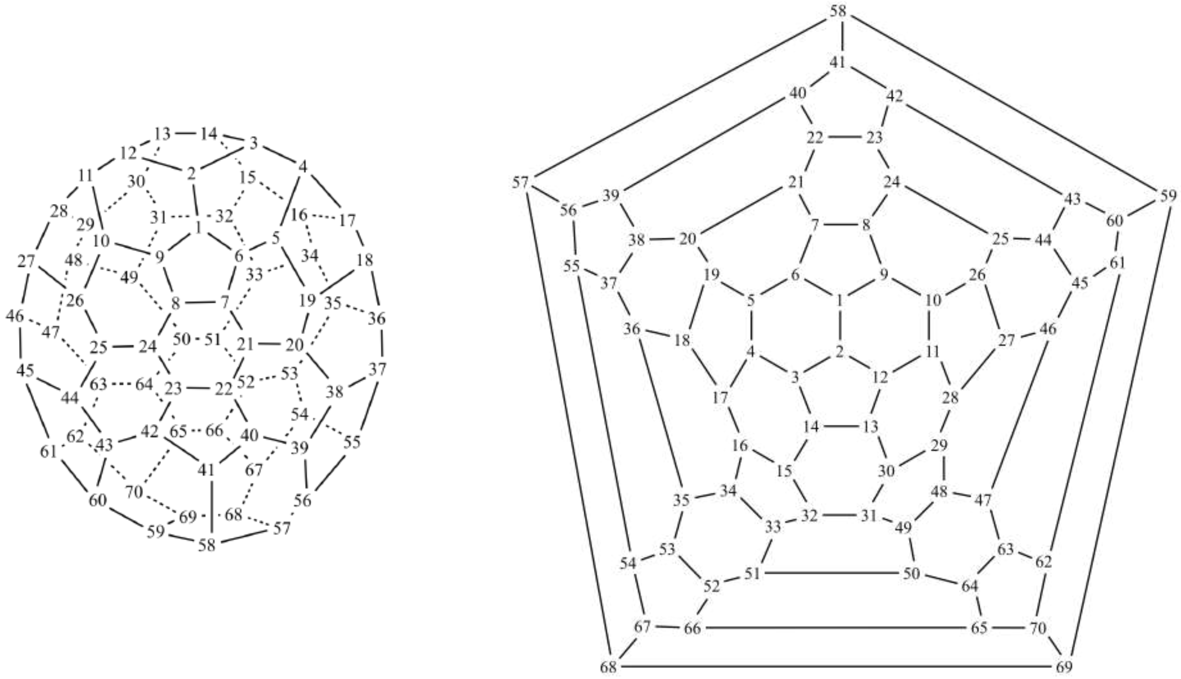
3-D Representation Schlegel representation

(C_{70}-$D_{5h(6)}$)[5,6]fullerene (PIN; systematic numbering)



3-D Representation Schlegel representation

(C_{60}-I_h)fullerene (trivial numbering)



3-D Representation   Schlegel representation

$[C_{70}\text{-}D_{5h(6)}]$fullerene (trivial numbering)

Specific numberings of many other fullerene structures with rotational symmetry axes, including those with a discontiguous numbering pathway (according to systematic principles), and fullerenes with C_s and C_1 point group symmetry have been published (ref. 11).

P-27.4 STRUCTURALLY MODIFIED FULLERENES

P-27.4.0 Introduction
P-27.4.1 Homofullerenes
P-27.4.2 Norfullerenes
P-27.4.3 Secofullerenes
P-27.4.4 Cyclofullerenes
P-27.4.5 Combination of structure-modifying operations

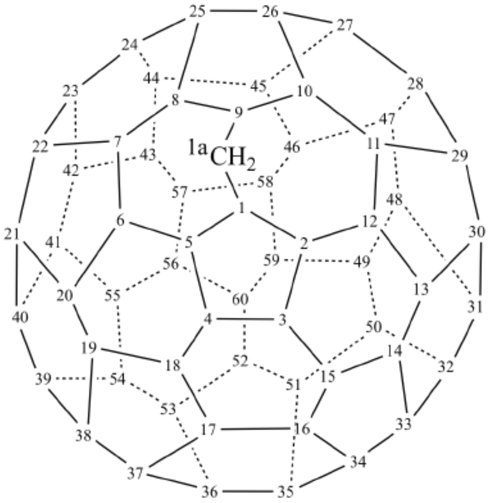
P-27.4.0 Introduction

The addition or removal of carbon atoms in a given fullerene does not create a new fullerene system described by a new number of carbon atoms and point group symbol, but is described by modifying the name of the unmodified fullerene using a nondetachable prefix, 'homo' or 'nor', respectively. In this way, fullerenes are parent structures analogous to fundamental structures used in the nomenclature of natural products (see Chapter P-10). Similarly, the cleavage of a bond or the formation of new bonds in specific situations is expressed by using the nondetachable prefixes 'seco' and 'cyclo', respectively, which are also used in the nomenclature of natural products. Contrary to the defined limited use of the prefixes 'homo', 'nor', 'seco', and 'cyclo' in the nomenclature of natural products, there is no such defined limitation in fullerene nomenclature.

P-27.4.1 Homofullerenes

The replacement of a carbon-carbon bond of a fullerene by a methylene ($–CH_2–$) group is described by attaching the nondetachable prefix 'homo' to the name of the parent fullerene. The original numbering of the parent fullerene is retained. The location of the homo operation is described by a compound locant formed according to the method devised for insertion of a methylene group into a bond connector of a fundamental structure in the nomenclature of natural products (see P-101.3.2). The addition of two or more methylene groups is indicated by multiplicative prefixes 'di', 'tri', etc. placed at the front of the prefix 'homo'. The compound locant is formed by adding the letter 'a' ('b', 'c', etc. if more than one methylene group replaces the bond) to the pair of locants which are the lowest locants consistent with the numbering of the fullerene, and enclosing the higher number in parentheses, for example '1(9)a'. Such compound locants must be used as locants in the names of the parent compounds, but, where there is no ambiguity, simple locants formed by adding the letter 'a' to the lowest locant, such as '1a' for the case above, may be used in structural formulas and for citation of substituents. Locants to denote the addition of methylene group(s) are differently used in the nomenclature of natural products (see P-101.3.2). Locants used by CAS are also different and must not be used to describe the replacement by methylene groups in preferred IUPAC names of fullerenes (see Fu-4.1, ref. 10).

Example:



1(9)aH-1(9)a-homo(C_{60}-I_h)[5,6]fullerene (PIN)

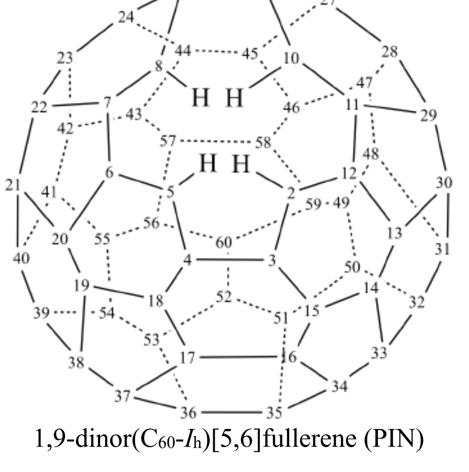
P-27.4.2 Norfullerenes

The nondetachable prefix ‘nor’ describes the deletion of one carbon atom from a fullerene structure; however, bonds attached to the atom removed are not reconnected as is the case in the nomenclature of natural products (see P-101.3.1.1). As a result, the connectivity of remaining atoms may be reduced from three to two, which requires the presence of hydrogen atoms. An even number of hydrogen atoms is implied in the name; if there is an odd number, one is expressed as indicated hydrogen because one carbon atom has changed from sp^2 to sp^3 hybridization. A connectivity of three may be satisfied by a heteroatom such as nitrogen or boron and a connectivity of two by a heteroatom such as oxygen or sulfur; these heteroatoms are introduced in a separate operation. Locants for the atoms must be as low as possible. The deletion of two or more carbon atoms is indicated by multiplicative prefixes ‘di’, ‘tri’, etc. placed at the front of the prefix ‘nor’.

It would not be helpful to set a precise number of carbon atoms that can be removed by the ‘nor’ operation for preferred IUPAC names; eventually, systematic ring nomenclature would provide a name which would be easier to understand than a polynorfullerene name. A realistic figure would depend much on whether blocks of carbon atoms or isolated carbon atoms are being removed. For the use of nor in the generation of preferred IUPAC fullerene names see P-52.2.6.1.

The use of the ‘nor’ prefix in the nomenclature of natural products is not the same and must not be used in, or adapted to, fullerene nomenclature.

Example:



1,9-dinor(C_{60}-I_h)[5,6]fullerene (PIN)

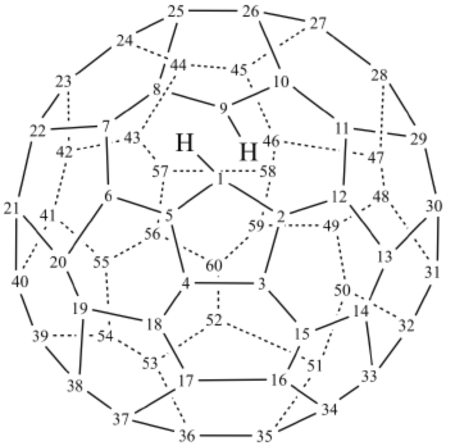
P-27.4.3 Secofullerenes

The nondetachable prefix ‘seco’ indicates the cleavage of one fullerene bond. Numbering of the parent fullerene is retained; where there is a choice, lowest possible locants are used to describe the seco operation. The valence requirements of the resulting carbon atoms with a connectivity of two are satisfied by hydrogen atoms following rearrangement of the double bonds. The hydrogen atoms are implied in the name of the secofullerene. The cleavage of two or more bonds is indicated by multiplicative prefixes ‘di’, ‘tri’, etc. placed at the front of the prefix ‘seco’.

It would not be helpful to set a precise number of bonds that can be cleaved by the ‘seco’ operation for preferred IUPAC names; eventually, systematic ring nomenclature would provide a name which would be easier to understand than a polysecofullerene name. A realistic figure would depend much on which bonds of the parent fullerene are being cleaved. For the generation of preferred IUPAC secofullerene names, see P-52.2.6.2.

The use of the ‘seco’ prefix in the nomenclature of natural products is not the same and must not be used in, or adapted to, fullerene nomenclature.

Example:



1,9-seco(C$_{60}$-*I*$_h$)[5,6]fullerene (PIN)

P-27.4.4 Cyclofullerenes

The nondetachable prefix ‘cyclo’ indicates the formation of a bond between two atoms of a modified fullerene or multifullerene structure. It almost always occurs in combination with one or more of the structure-modifying prefixes ‘homo’, ‘nor’, and ‘seco’. The formation of two or more bonds, when required, is indicated by multiplicative prefixes ‘di’, ‘tri’, etc. placed at the front of the prefix ‘cyclo’. No single fullerene is yet known that uses only ‘cyclo’. See the example under P-27.4.5.

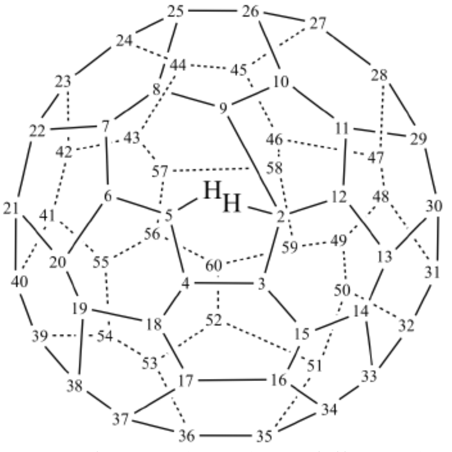
P-27.4.5 Combination of structure-modifying operations

When more than one operation has been performed in a fullerene structure, the prefixes designating these operations are cited in names in the order ‘cyclo’, ‘seco’, ‘homo’, and ‘nor’ in front of the name of the fullerene. This is the reverse order that the operation indicated by the prefix has for assignment of lowest locants. ‘Nor’ prefixes are considered first for lowest locants and ‘homo’ prefixes are senior to ‘seco’ and ‘cyclo’ for lowest locants, since ‘homo’ locants may be needed for the latter operations. Locants for ‘cyclo’ and ‘seco’ prefixes are determined by the lowest set of locants, then by the order of citation of the locants in the name.

It would not be helpful to set a precise number of operations that can be performed on a parent fullerene structure for generation of preferred IUPAC names; eventually, systematic ring nomenclature would provide a name which would be easier to understand than a polysecofullerene name. A realistic number would depend much on the type of operations combined. For the use of structure-modifying prefixes in generating preferred IUPAC fullerene names, see P-52.2.6.

The rules for combinations of structure-modifying prefixes used in the nomenclature of natural products are not the same and must not be used in, or adapted to, fullerene nomenclature.

Example:

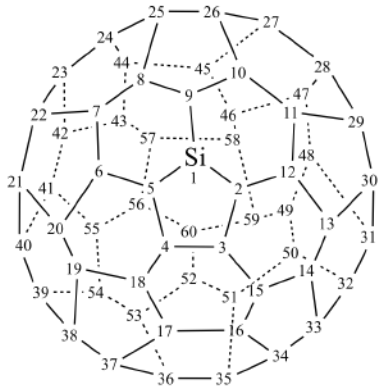


2*H*-2,9-cyclo-1-nor(C_{60}-I_h)[5,6]fullerene (PIN)

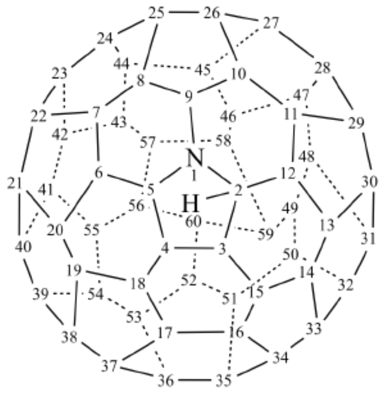
P-27.5 REPLACEMENT OF SKELETAL ATOMS

P-27.5.1 Fullerenes in which carbon atoms have been replaced by one or more heteroatoms are called ‘heterofullerenes’. Skeletal replacement (‘a’) nomenclature is used to name fullerenes in which carbon atoms have been replaced by heteroatoms having standard bonding numbers according to the ‘a’ prefixes of organic replacement nomenclature (see P-15.4) or bonding numbers indicated by the λ-convention (see P-14.1). The parent name is ‘fullerene’ if double bonds are present or possible in the parent fullerene; if double bonds are not possible, the parent name is ‘fullerane’. The heteroatoms include all elements capable of being tricoordinate, including metals and semimetals. Replacement names for fullerenes in which all carbon atoms have been replaced by the same or different heteroatoms are preselected names (see P-12.2). Replacement of carbon atoms by trivalent heteroatoms may result in the need for indicated hydrogen that receives lowest possible locants.

Examples:



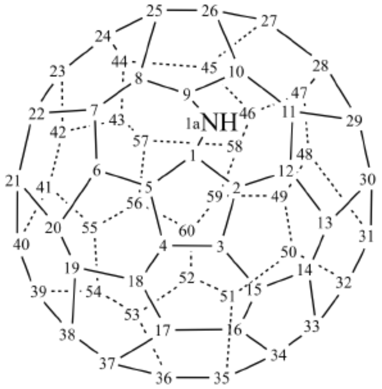
sila(C_{60}-I_h)[5,6]fullerene (PIN)



2*H*-1-aza(C_{60}-I_h)[5,6]fullerene (PIN)

P-27.5.2 When ‘homo’, ‘nor’, ‘seco’, or ‘cyclo’ prefixes co-occur with skeletal replacement terms, such as ‘oxa’ or ‘aza’, the replacement prefixes are cited in names in order of their seniority before structure-modifying prefixes. Structure-modifying prefixes are assigned low locants over replacement prefixes.

Example:



1a*H*-1a-aza-1(9)a-homo(C_{60}-I_h)[5,6]fullerene (PIN)

P-27.6 ADDITION OF RINGS AND RING SYSTEMS TO FULLERENES

Addition of rings or ring systems to a fullerene is expressed as an ortho fusion operation, a bridging operation, or as a spirofusion operation as previously described in this Chapter.

P-27.6.1 Fullerenes and modified fullerenes *ortho* fused to organic rings or ring systems
P-27.6.2 Bridged fullerenes
P-27.6.3 Spiro fullerenes

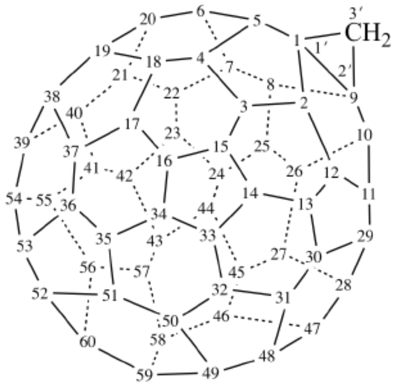
P-27.6.1 Fullerenes and modified fullerenes *ortho* fused to organic rings or ring systems

Fullerenes or modified fullerenes that share an adjacent pair of atoms with an organic ring or ring system are named by adapting the principles of fusion nomenclature described in Section P-25. As in normal organic fused ring systems, the pair of atoms shared by the fullerene or modified fullerene and the organic ring or ring system is regarded as part of both components. However, unlike normal fused systems, each component retains its own bonding pattern and numbering. Because of the nature of bonding in fullerenes, the fusion bond is always a single bond and the fusion atoms cannot accept an 'exo' double bond. After fusion, nonfullerene components other than alicyclic bi- and polycyclic ring systems have the maximum number of noncumulative double bonds and indicated hydrogen is cited as needed.

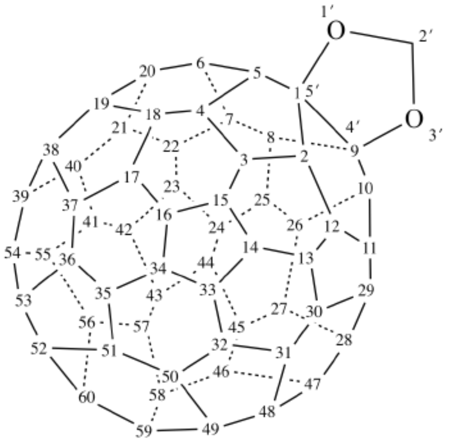
Organic ring systems, including monocyclic rings and all polycyclic ring systems except spiro ring systems, are always cited as prefixes to the name of the fullerene or modified fullerene which is always the parent component. Each system retains its own name and numbering, both for indicating fusion sites and for indicating positions of substitution. The fullerene or modified fullerene locants are always unprimed, and primes are added to the fused organic ring or ring systems in the order described below. The fusion is described by citing the primed locants of the organic ring or ring system component and the unprimed locants of the fullerene or modified fullerene in that order, enclosed in brackets and separated by a colon. Locants for monocyclic hydrocarbons are omitted in preferred IUPAC names.

The methodology used to name fused derivatives of fullerenes is also used for naming fused fundamental structures in the nomenclature of natural products (see P-101.5). It is important to note that it must be integrally applied as described to generate IUPAC names. CAS names are different and more in line with the normal fusion operation in which the parent component is the senior ring or ring system. When this approach must be used, CAS names of fullerenes and modified fullerenes must be used. Furthermore, it is possible to replace fusion operations by bridging operations, as for example when the ring component is a cyclopropane or an oxirene ring. In these cases, bridging by using the bridging prefixes 'methano' or 'epoxy' (see P-25.4) can be an important alternative; this method was recommended in the preliminary survey (see ref. 25) and can be used in general nomenclature.

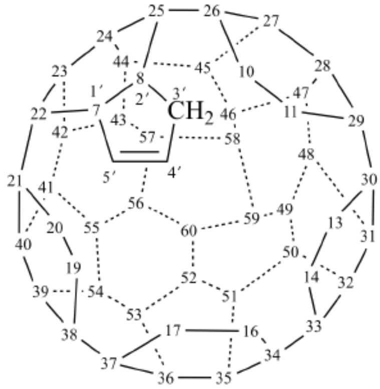
Examples:



3′*H*-cyclopropa[1,9](C_{60}-I_h)[5,6]fullerene (PIN)
1,9-methano(C_{60}-I_h)[5,6]fullerene (see P-27.6.2)



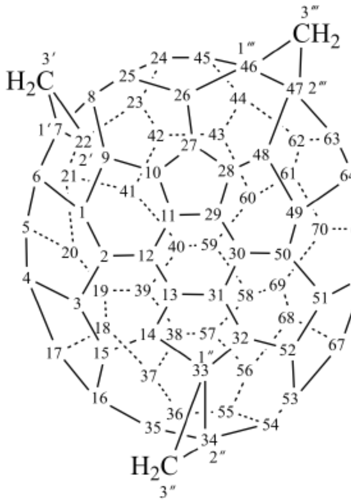
[1,3]dioxolo[4′,5′:1,9](C_{60}-I_h)[5,6]fullerene (PIN)
1,9-(oxymethyleneoxy)(C_{60}-I_h)[5,6]fullerene (see P-27.6.2)



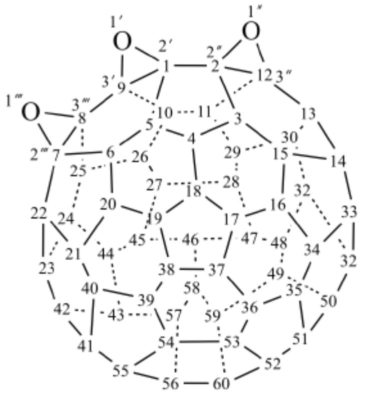
3′*H*-cyclopenta[7,8]-1,2,3,4,5,6,9,12,15,18-decanor(C_{60}-I_h)[5,6]fullerene (PIN)
7,8-(prop-1-en-1,3-diyl)-1,2,3,4,5,6,9,12,15,18-decanor(C_{60}-I_h)[5,6]fullerene (see P-27.6.2)

When two or more of the same nonfullerene components are fused to a fullerene, primes are assigned according to the increasing value of the lower fullerene fusion locant. When different nonfullerene components are attached to a fullerene, primes are assigned in the alphanumerical order of the fusion prefix in the name reading from left to right, respecting the criterion for multiples of the same nonfullerene component just given. This methodology also applies to rings and ring systems fused to modified fullerenes.

Examples:



3′*H*,3″*H*,3‴*H*-tricyclopropa[7,22:33,34:46,47](C_{70}-$D_{5h(6)}$)[5,6]fullerene (PIN)
7,22:33,34:46,47-tris(methylene)(C_{70}-$D_{5h(6)}$)[5,6]fullerene (see P-27.6.2)

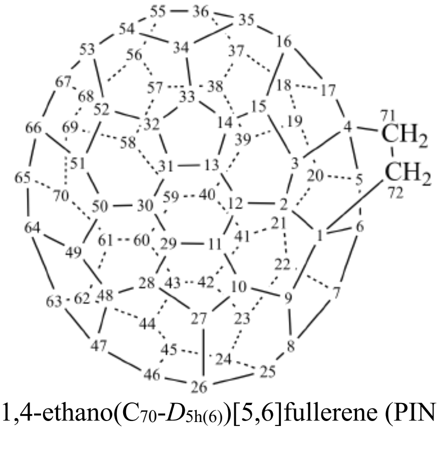


tris(oxireno)[2′,3′:1,9;2″,3″:2,12;2‴,3‴:7,8](C_{60}-I_h)[5,6]fullerene (PIN)
1,9:2,12:7,8-tris(oxy)(C_{60}-I_h)[5,6]fullerene (see P-27.6.2)

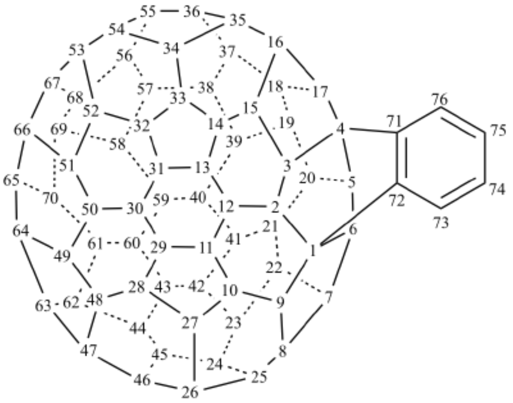
P-27.6.2 Bridged fullerenes

Bridges between nonadjacent atoms of a fullerene or modified fullerene are named and numbered according to established principles and rules for bridged fused ring systems (see P-25.4). Numbering of bridging atoms begins with the number following the highest number of the fullerene and starts with the atom adjacent to the fullerene atom with the higher locant number. Bridges between rings fused to fullerene and a parent fullerene, between two different rings fused to the same fullerene, or between two or more fullerenes joined by fused rings or ring systems are named using established bridge prefix names, but numbering begins with the bridge atom adjacent to the fused component with the least primed numbers and continues from this atom.

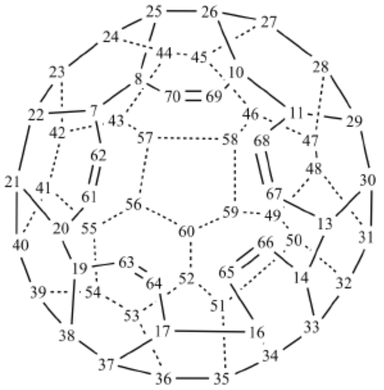
Examples:



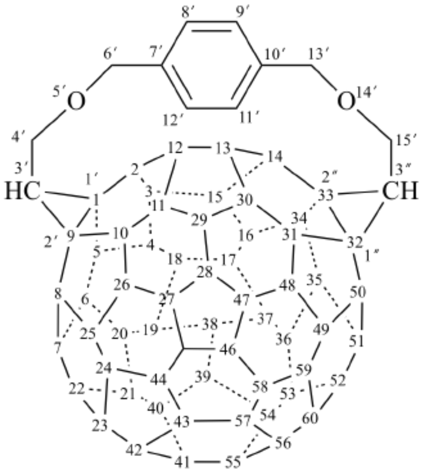
1,4-ethano(C_{70}-$D_{5h(6)}$)[5,6]fullerene (PIN)


55 — 36 — 35
54 34 37 16
53 56 18 17
67 68 57 38 33
66 69 52 32 14 15 39 19 4 71 76 75
58 31 13 3
65 51 20 5
70 50 30 59 40 12 2 72 74
64 61 60 29 11 41 21 1 6 73
49 22
63 62 48 28 43 42 10 9 7
44 27 23
47 45 24 8
46 26 25

1,4-[1,2]benzeno(C_{70}-$D_{5h(6)}$)[5,6]fullerene (PIN)


25 26 27
24 44 45 28
23 8 10
70 = 69
22 7 11 29
42 43 57 58 46 47
62 68 48
21 41 61 67 30
20 55 56 60 59 49 13
40 66 50 31
19 63 64 52 65 14 32
39 54 53 51
38 17 16 33
37 34
36 35

7,20:8,10:11,13:14,16:17,19-pentaetheno-1,2,3,4,5,6,9,12,15,18-decanor(C_{60}-I_h)[5,6]fullerene (PIN)


8′ 9′
6′ 7′ 10′ 13′
5′ O O 14′
12′ 11′
4′ 15′
3′ 3″
HC CH
1′ 2″
2′ 1″
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20
21 22 23 24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40
41 42 43 44 45 46 47 48 49 50 51 52 53 54 55 56 57 58 59 60

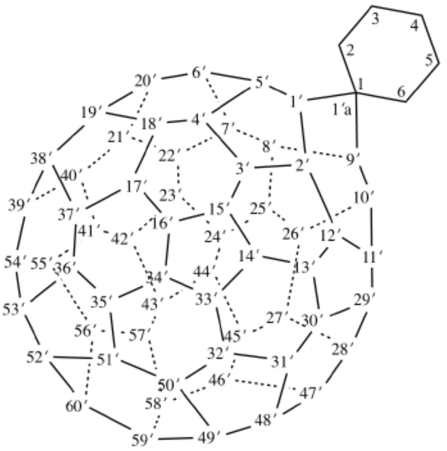
3′*H*,3″*H*-3′,3″-(methanooxymethano[1,4]benzenomethanooxymethano)dicyclopropa-[1,9:32,33](C_{60}-I_h)[5,6]fullerene (PIN)

1,9:32,33-[ethane-1,1,2-triyloxymethylene(1,4-phenylene)methyleneoxyethane-1,2,2-triyl)(C_{60}-I_h)[5,6]fullerene

P-27.6.3 Spiro fullerenes

Fullerenes cannot themselves form spiro compounds directly due to their specific connectivity and, as mentioned earlier, spiro ring systems are not fused to fullerenes. Spiro fullerenes formed from homofullerenes and fullerenes fused to organic ring systems follow the normal procedure for naming organic spiro systems that contain at least one polycyclic ring system, as described in P-24.5. Spiro fullerene parent hydrides will not necessarily have unprimed numbers as locants, as the alphanumerical order is used to name this type of spiro compound.

Example:



spiro[cyclohexane-1,1′a-[1(9)a]homo(C_{60}-I_h)[5,6]fullerene] (PIN)

P-27.7 OTHER ASPECTS OF FULLERENE NOMENCLATURE

Part II of fullerene nomenclature, ref. 11, discusses rules for numbering a wide variety of fullerene structures:

(1) Fullerenes having at least one symmetry axis (C_n; n>1) and a contiguous helical numbering pathway

(2) Fullerenes having at least one symmetry axis (C_n; n>1) but no contiguous helical numbering pathway

(3) Fullerenes belonging to the C_s point group and having a contiguous helical numbering pathway

(4) Fullerenes belonging to the C_i or C_1 point groups and having a contiguous helical numbering pathway

P-28 RING ASSEMBLIES

P-28.0 Introduction
P-28.1 Definitions
P-28.2 Ring assemblies of two identical cyclic systems
P-28.3 Unbranched ring assemblies of three through six identical cyclic systems
P-28.4 Ring assemblies of identical cyclic systems modified by skeletal replacement (‘a‘) nomenclature
P-28.5 Ring assembles of more than six identical cyclic systems
P-28.6 Branched ring assemblies of identical cyclic systems
P-28.7 Ring assemblies of nonidentical cyclic systems

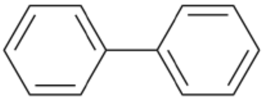
P-28.0 INTRODUCTION

Assemblies of cyclic parent hydrides linked by single or double bonds are described in this Section. They are named by using the so-called ‘Latin multiplying prefixes’, ‘bi’, ‘ter’, ‘quater’, etc., to indicate the number of rings or ring systems in the assembly.

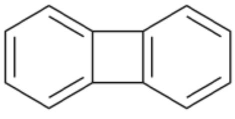
Names of substituent groups described further in Section P-29 are used in this Section.

P-28.1 DEFINITIONS

Two or more cyclic systems (single rings or fused systems, alicyclic von Baeyer systems, spiro systems, phane systems, fullerenes) that are directly joined to each other by single or double bonds are called ‘ring assemblies’ when the number of such direct ring junctions is one less than the number of cyclic systems involved.

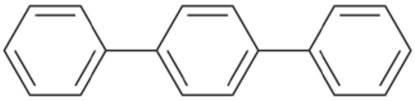


a ring assembly

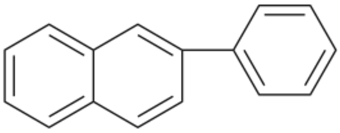


a fused ring system

Ring assemblies are composed of identical cyclic systems (rings or ring systems); assemblies of nonidentical cyclic systems (rings or ring systems) are not called ring assemblies for the purposes of organic nomenclature, for example:



three identical rings (a ring assembly)



two different ring systems

P-28.2 RING ASSEMBLIES OF TWO IDENTICAL CYCLIC SYSTEMS

P-28.2.1 Ring assemblies with a single bond junction

Assemblies of two identical cyclic systems joined by a single bond are named by one of two methods:

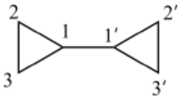
(1) by placing the prefix 'bi' (see P-14.2.3) before the name of the corresponding parent hydride enclosed in parentheses, if necessary. Parentheses are used to avoid confusion with von Baeyer names;

(2) by placing the prefix 'bi' (see P-14.2.3) before the name of the corresponding substituent group (for names of substituent groups, see P-29), enclosed in parentheses, if necessary.

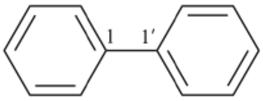
Each cyclic system is numbered in the traditional way, one with unprimed locants, the other with primed locants. Lowest possible locants must be used to denote the positions of attachment. These locants must be cited in preferred IUPAC names; they can be omitted in general nomenclature when no ambiguity would result.

The name biphenyl is retained as 1,1′-biphenyl.

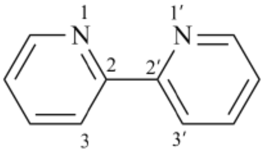
Examples:



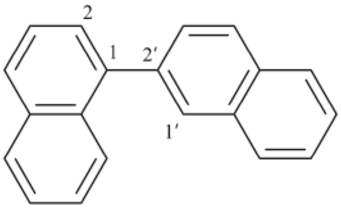
(1) 1,1′-bi(cyclopropane) (PIN)
(2) 1,1′-bi(cyclopropyl)



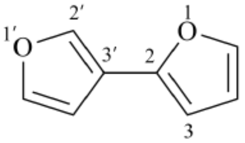
(2) 1,1′-biphenyl (PIN)
biphenyl



(1) 2,2′-bipyridine (PIN)
(2) 2,2′-bipyridyl



(1) 1,2′-binaphthalene (PIN)
(2) 1,2′-binaphthyl

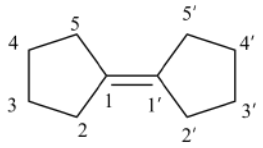


(1) 2,3′-bifuran (PIN)
(2) 2,3′-bifuryl

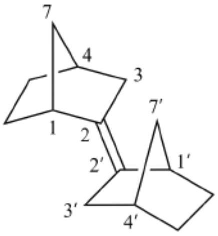
P-28.2.2 Ring assemblies with a double bond junction

When two cyclic systems are linked by a double bond, method (2) described in P-28.2.1 is the only recommended method. Method (2) has also been used in which the presence of a double bond is indicated by the Greek letter Δ and the point of attachment of the ring is given by superscript locant numbers. This method is not continued in these recommendations; accordingly, ring assemblies of three or more identical cyclic systems interconnected by double bonds must be named by other methods (see P-31).

Examples:



1,1′-bi(cyclopentylidene) (PIN)
(not $\Delta^{1,1'}$-bicyclopentylidene)



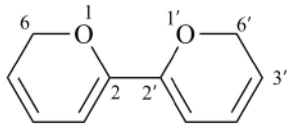
2,2′-bi(bicyclo[2.2.1]heptanylidene) (PIN)
(not $\Delta^{2,2'}$-bicyclo[2.2.1]heptanylidene)

P-28.2.3 Indicated hydrogen of components in two-component ring assemblies is named and numbered according to P-58.2.1, ignoring the indicated hydrogen atoms of the component rings or ring systems. The maximum number of noncumulative double bonds is then added taking into account the junction positions. Any remaining saturated ring positions are designated as indicated hydrogen, placed together with the appropriate locant(s) at the front of the name of the assembly.

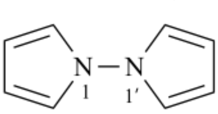
> The citation of indicated hydrogen, if needed, at the front of the name of the ring assembly is a change from its position in previous editions (refs. 1 and 2) where it was kept with the name of the individual ring, for example, 2,2′-bi-2*H*-pyran.

Note: Citing the indicated hydrogen in front of the name of the ring assembly follows the method now adopted for bridged fused systems (see P-25.7.1.3.2) and spiro ring systems (see P-24.3.2). This method allows more assemblies of rings to be treated as ring assemblies, for example, 1*H*,2′*H*-2,4′-biindene. The advantages of this method become more obvious when naming derivatives requiring a divalent substituent group suffix, such as a ketone.

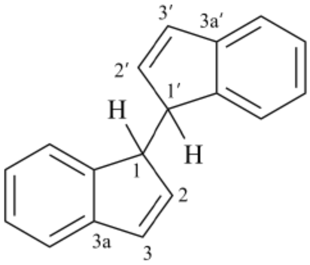
Examples:



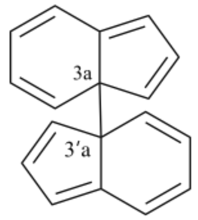
6*H*,6′*H*-2,2′-bipyran (PIN)
(not 2,2′-bi-6*H*-pyran)



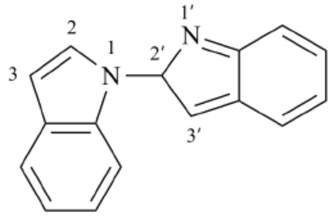
1,1′-bipyrrole (PIN)
(no indicated hydrogen needed)
(not 1,1′-bi-1*H*-pyrrole)



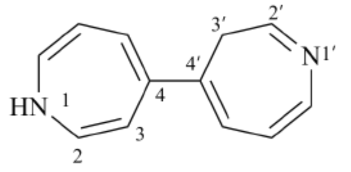
1*H*,1′*H*-1,1′-biindene (PIN)
(not 1,1′-bi-1*H*-indene)



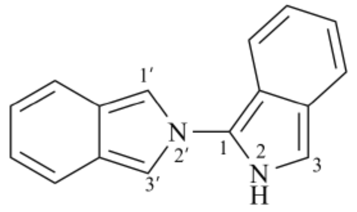
3a,3′a-biindene (PIN)
(no indicated hydrogen needed)
(not 3a,3′a-bi-3a*H*-indene)



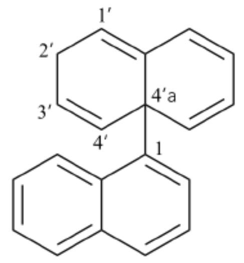
2′*H*-1,2′-biindole (PIN)



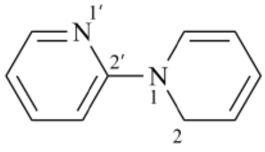
1*H*,3′*H*-4,4′-biazepine (PIN)



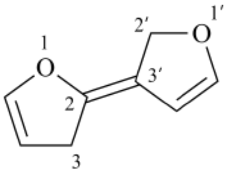
2*H*-1,2′-biisoindole (PIN)



2′*H*-1,4′a-binaphthalene (PIN)



2*H*-1,2′-bipyridine (PIN)



2′*H*,3*H*-2,3′-bifuranylidene (PIN)

P-28.3 UNBRANCHED RING ASSEMBLIES OF THREE THROUGH SIX IDENTICAL CYCLIC SYSTEMS

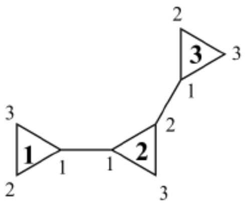
P-28.3.1 Unbranched ring assemblies consisting of three or more identical cyclic systems are named by placing the appropriate numerical Latin-based (see P-14.2.3) prefix, ‘ter’, ‘quater’, ‘quinque’, etc., before the name of the parent hydride corresponding to the repeating unit. Indicated hydrogen is applied as described above for two-component ring assemblies (see P-28.2.3).

Exceptionally, ring assemblies composed of three or more benzene rings are named by using the term ‘phenyl’. Each cyclic system of the assembly is numbered consecutively and each ring or ring system is numbered in its usual way provided the lowest locant set is selected and, if a choice remains, in the order of citation in the name. Composite locants (see P-14.3.1) are formed by citing the locants denoting positions in each ring or ring system as superscripts to the locants indicating the position of a cyclic system in the assembly (ref. 26). Locants indicating points of attachment are placed before the name of the assembly in ascending order; locants denoting junctions are separated by a comma and sets of junction locants are separated by a colon.

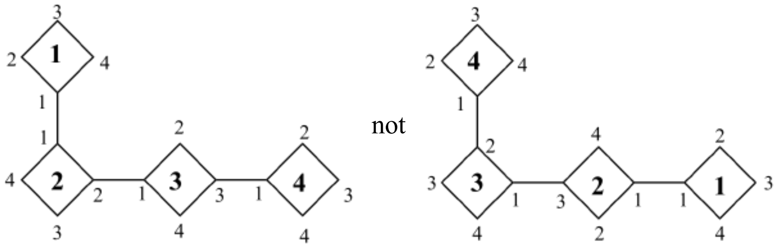
> This is a new numbering system recommended for ring assemblies consisting of more than two rings or ring systems. The new system, which uses composite locants composed of primary locants and superscript numbers attached to them as described above, is recommended for preferred IUPAC names. The numbering method using serially primed locants used in earlier recommendations (refs. 1 and 2) may be used in general nomenclature.

Note: The elimination of primed locants for preferred IUPAC names is intended to improve the perception of the relationship between structures and names. The new numbering system for preferred IUPAC names is similar to that recommended in phane nomenclature (see P-26.1). For example, two alternative names are 1,1′:2′,1″-tercyclopropane and $1^1,2^1:2^2,3^1$-tercyclopropane, where the primary locants 1,2,3 correspond to the three rings of the assembly, and the superscript locants pertain to the locants of the points of attachment of the three rings.

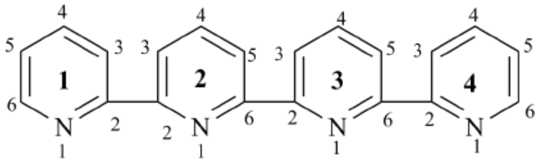
Examples:



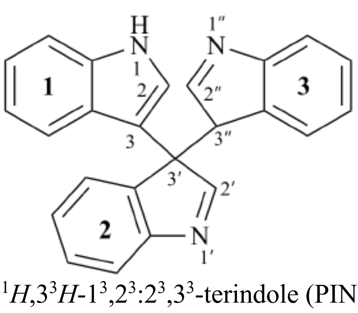
$1^1,2^1:2^2,3^1$-tercyclopropane (PIN)
1,1′:2′,1″-tercyclopropane



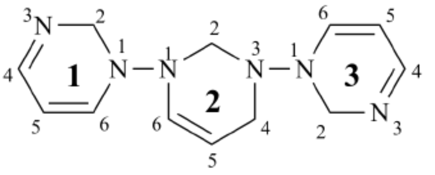
$1^1,2^1:2^2,3^1:3^3,4^1$-quatercyclobutane (PIN)
(not $1^1,2^1:2^3,3^1:3^2,4^1$-quatercyclobutane;
the locant set $1^1,2^1:2^2,3^1:3^3,4^1$ is lower than the locant set $1^1,2^1:2^3,3^1:3^2,4^1$)
1,1′:2′,1″:3″,1‴-quatercyclobutane
(not 1,1′:3′,1″:2″,1‴-quatercyclobutane;
the locant set 1,1′:2′,1″:3″,1‴ is lower than 1,1′:3′,1″:2″,1‴)



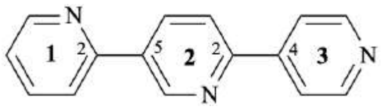
$1^2,2^2:2^6,3^2:3^6,4^2$-quaterpyridine (PIN)
2,2′:6′,2″:6″,2‴-quaterpyridine



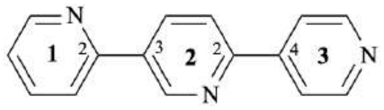
$1^1H,3^3H-1^3,2^3:2^3,3^3$-terindole (PIN)
1*H*,3″*H*-3,3′:3′,3″-terindole



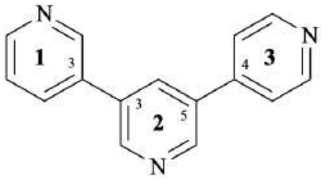
1^2*H*,2^2*H*,2^4*H*,3^2*H*-$1^1,2^1{:}2^3,3^1$-terpyrimidine (PIN)
2*H*,2′*H*,2″*H*,4′*H*-1,1′:3′,1″-terpyrimidine



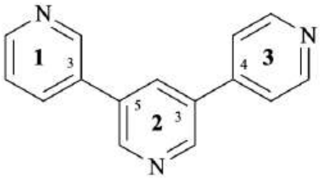
not



$1^2,2^5{:}2^2,3^4$-terpyridine (PIN)
(not $1^2,2^3{:}2^6,3^4$-terpyridine);
the locant set $1^2,2^2,2^5,3^4$ is lower than the locant set $1^2,2^3,2^6,3^4$)
2,5′:2′,4″-terpyridine
(not 2,3′:6′,4″-terpyridine
the locant set 2,2′,4″,5′ is lower than the locant set 2,3′,4″,6′)



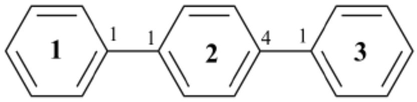
not



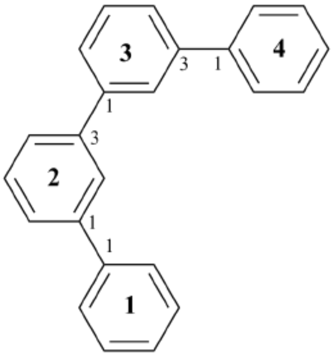
$1^3,2^3{:}2^5,3^4$-terpyridine (PIN)
(not $1^3,2^5{:}2^3,3^4$-terpyridine);
both locant sets are the same but $1^3,2^3{:}2^5,3^4$ is lower than $1^3,2^5{:}2^3,3^4$ in the order of citation.
3,3′:5′,4″-terpyridine
(not 3,5′:3′,4″-terpyridine
both locant sets are the same but 3,3′:5′,4″ is lower than 3,5′:3′,4″ in the order of citation.

P-28.3.2 As exceptions to the use of parent hydride names, ring assemblies of three through six benzene rings are named by method (2) as given in P-28.2.1, yielding names such as terphenyl, quaterphenyl, etc.

Examples:



$1^1,2^1{:}2^4,3^1$-terphenyl (PIN)
1,1′:4′,1″-terphenyl
(not *p*-terphenyl)

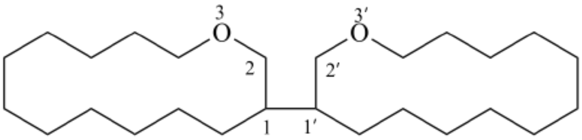


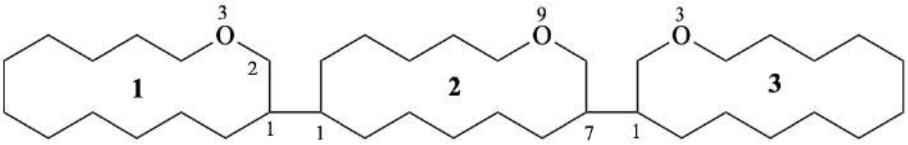
$1^1,2^1{:}2^3,3^1{:}3^3,4^1$-quaterphenyl (PIN)
1,1′:3′,1″:3″,1‴-quaterphenyl
(not *m*-quaterphenyl)

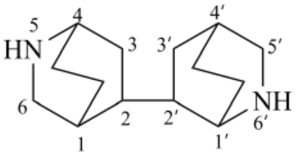
P-28.4 RING ASSEMBLIES COMPOSED OF IDENTICAL CYCLIC SYSTEMS MODIFIED BY SKELETAL REPLACEMENT (‘a’) NOMENCLATURE

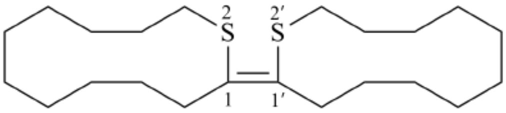
P-28.4.1 Assemblies composed of identical heterocyclic compounds are named by using the names of parent hydrides, except in the case of heterocyclic compounds of the von Baeyer type and of monocyclic compounds having more than 10 members that are named by using skeletal replacement (‘a’) nomenclature. In the latter cases, the ‘a’ prefixes are placed at the front of the name of the hydrocarbon ring assembly.

Examples:


3,3′-dioxa-1,1′-bi(cyclotetradecane) (PIN)

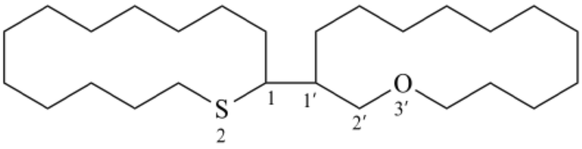

$1^3,2^9,3^3$-trioxa-$1^1,2^1{:}2^7{:}3^1$-tercyclotetradecane (PIN)
(not $1^3,2^{13},3^3$-trioxa-$1^1,2^1{:}2^7{:}3^1$-tercyclotetradecane; $1^3,2^9,3^3$ is lower than $1^3,2^{13},3^3$)
3,3″,9′-trioxa-1,1′:7′,1″-tercyclotetradecane
(not 3,3″,13′-trioxa-1,1′:7′,1″-tercyclotetradecane; 3,3″,9′ is lower than 3,3″,13′)

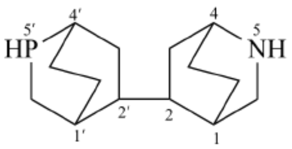

5,6′-diaza-2,2′-bi(bicyclo[2.2.2]octane) (PIN)


2,2′-dithia-1,1′-bi(cyclododecylidene) (PIN)

P-28.4.2 Since hydrocarbon ring assemblies are the parent structures for the application of skeletal replacement (‘a’) nomenclature, heteroatoms do not need to be identical or present in the same number. When heteroatoms of different elements are present, normal skeletal replacement (‘a’) nomenclature is used to name the heterocycles. Low locants are assigned to heteroatoms as a set, then in the order: O > S > Se > Te > N > P > As > Sb > Bi > Si > Ge > Sn > Pb > B > Al > Ga > In > Tl.

Examples:

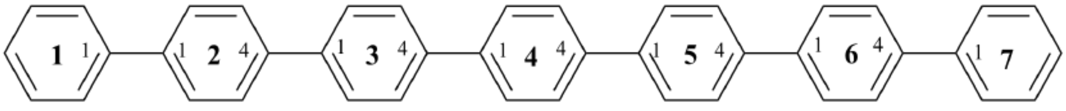

3′-oxa-2-thia-1,1′-bi(cyclotetradecane) (PIN)
[not 3-oxa-2′-thia-1,1′-bi(cyclotetradecane);
the locant set 2,3′ is lower than 2′,3]

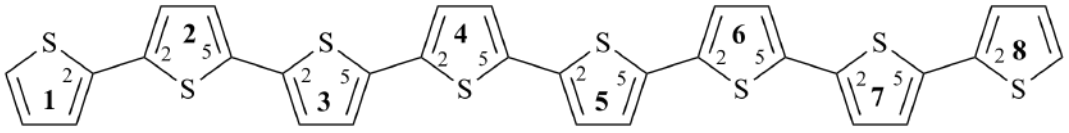

5-aza-5′-phospha-2,2′-bi(bicyclo[2.2.2]octane) (PIN)
[not 5′-aza-5-phospha-2,2′-bi(bicyclo[2.2.2]octane);
the locant 5 is lower than 5′, and the prefix ‘aza’ has priority to be assigned the lower locant]

P-28.5 RING ASSEMBLES OF MORE THAN SIX IDENTICAL CYCLIC SYSTEMS

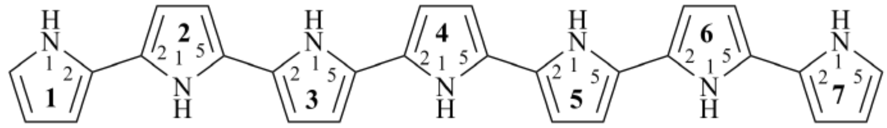
Preferred IUPAC names for ring assemblies of more than six identical cyclic systems are generated using the principles of phane nomenclature (see P-26). Any of the methods discussed above (see P-28.2.1, P-28.3.1, P-28.3.2), as appropriate, can be used in general IUPAC nomenclature.

Examples:


1,7(1),2,3,4,5,6(1,4)-heptabenzenaheptaphane (PIN)
$1^1,2^1{:}2^4,3^1{:}3^4,4^1{:}4^4,5^1{:}5^4,6^1{:}6^4,7^1$-septiphenyl
1,1′:4′,1″:4″,1‴:4‴,1‴′:4‴′,1‴″:4‴″,1‴‴-septiphenyl



1,8(2),2,3,4,5,6,7(2,5)-octathiophenaoctaphane (PIN)
$1^{2},2^{2}:2^{5},3^{2}:3^{5},4^{2}:4^{5},5^{2}:5^{5},6^{2}:6^{5},7^{2}:7^{5},8^{2}$-octithiophene
2,2′:5′,2″:5″,2‴:5‴,2‴′:5‴′,2‴″:5‴″,2‴‴:5‴‴,2‴‴′-octithiophene

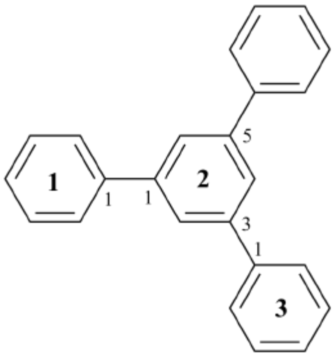


$1^{1}H,2^{1}H,3^{1}H,4^{1}H,5^{1}H,6^{1}H,7^{1}H$-1,7(2),2,3,4,5,6(2,5)-heptapyrrolaheptaphane (PIN)
$1^{1}H,2^{1}H,3^{1}H,4^{1}H,5^{1}H,6^{1}H,7^{1}H$-$1^{2},2^{2}:2^{5},3^{2}:3^{5},4^{2}:4^{5},5^{2}:5^{5},6^{2}:6^{5},7^{2}$-septipyrrole
1*H*,1′*H*,1″*H*,1‴*H*,1‴′*H*,1‴″*H*,1‴‴*H*-2,2′:5′,2″:5″,2‴:5‴,2‴′:5‴′,2‴″:5‴″,2‴‴-septipyrrole

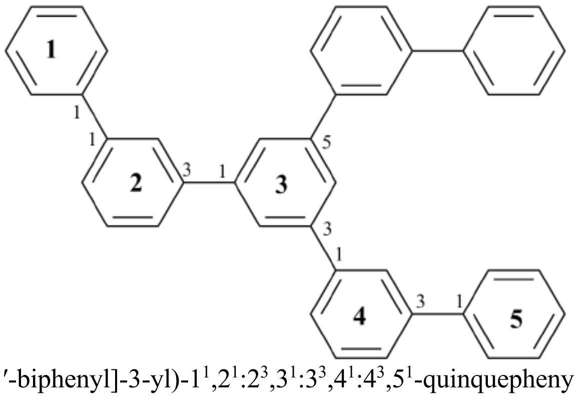
P-28.6 BRANCHED RING ASSEMBLIES OF IDENTICAL CYCLIC SYSTEMS

Preferred IUPAC names are formed by substituting into the longest unbranched assembly. The names of substituent groups are formed in accord with the methods described in P-29.3.5. If necessary, the criteria for selecting the principal chain are applied, namely, the longest chain, the lowest attachment locants in the order of citation, the maximum number of substituents, the lowest locants for substituents considered together, then alphanumerical order.

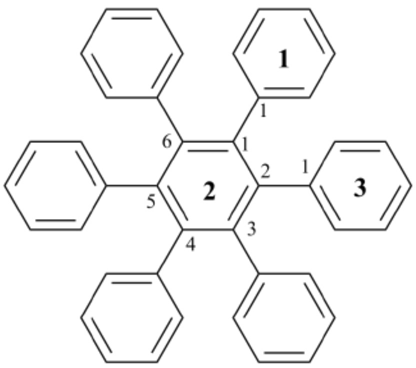
Examples:



2^{5}-phenyl-$1^{1},2^{1}:2^{3},3^{1}$-terphenyl (PIN)
5′-phenyl-1,1′:3′,1″-terphenyl

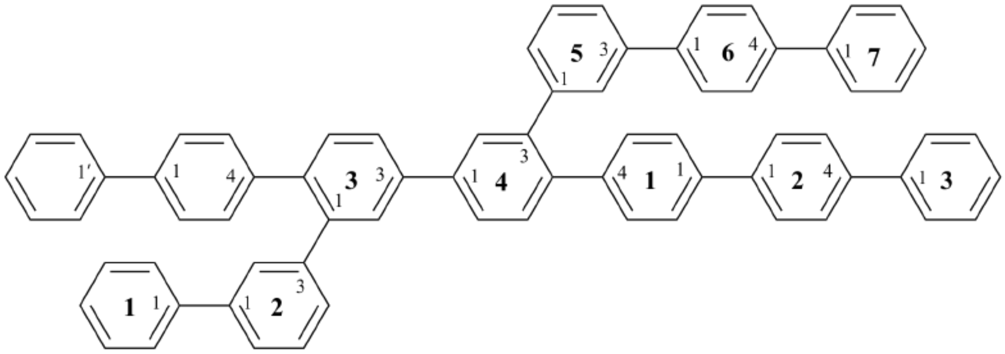


3^{5}-([1,1′-biphenyl]-3-yl)-$1^{1},2^{1}:2^{3},3^{1}:3^{3},4^{1}:4^{3},5^{1}$-quinquephenyl (PIN)
5″-([1,1′-biphenyl]-3-yl)-1,1′:3′,1″:3″,1‴:3‴,1‴′-quinquephenyl



$2^{3},2^{4},2^{5},2^{6}$-tetraphenyl-$1^{1},2^{1}:2^{2},3^{1}$-terphenyl (PIN)
(not $2^{2},2^{3},2^{5},2^{6}$-tetraphenyl-$1^{1},2^{1}:2^{4},3^{1}$-terphenyl
nor $2^{2},2^{4},2^{5},2^{6}$-tetraphenyl-$1^{1},2^{1}:2^{3},3^{1}$-terphenyl;
the locant set $1^{1},2^{1}:2^{2},3^{1}$ is lower than either $1^{1},2^{1}:2^{4},3^{1}$ or $1^{1},2^{1}:2^{3},3^{1}$)

3′,4′,5′,6′-tetraphenyl-1,1′:2′,1″-terphenyl
(not 2′,3′,5′,6′-tetraphenyl-1,1′:4′,1″-terphenyl
nor 2′,4′,5′,6′-tetraphenyl-1,1′:3′,1″-terphenyl;
the locant set 1,1′:2′,1″ is lower than either 1,1′:4′,1″ or 1,1′:3′,1″)



3^6-([1,1′-biphenyl]-4-yl)-4^4-([1^1,2^1:2^4,3^1-terphenyl]-1^4-yl)-1,7(1),2,3,4,5(1,3),6(1,4)-heptabenzenaheptaphane (PIN)
[not 3^2-([1,1′-biphenyl]-3-yl)-4^3-([1^1,2^1:2^4,3^1-terphenyl]-1^3-yl)-1,7(1),2,3,4,5,6(1,4)-heptabenzenaheptaphane;
the set of attachment locants (1,3)(1,3)(1,3)(1,3) for the superatom locants
2,3,4,5 is lower than (1,4)(1,4)(1,4)(1,4)]

P-28.7 RING ASSEMBLIES OF NONIDENTICAL CYCLIC SYSTEMS

Assemblies of cyclic systems that cannot be treated as ring assemblies as described above (P-28.2 and P-28.3) are simply assemblies of nonidentical cyclic systems and are named by substitutive nomenclature principles. Such cyclic hydrocarbon assemblies are discussed in Section P-61.2.2; and assemblies of nonidentical cyclic systems containing heteroatoms, such as Si, N, B, are considered in Section P-68. Phane nomenclature (see P-26), where applicable, is used to name ring assemblies composed of identical or nonidentical cyclic systems.

Ring assemblies of identical cyclic systems that are partially unsaturated or partially saturated can be modified either by the endings ‘ene’ or ‘yne’ (introduction of multiple bonds in saturated systems) or by using the prefixes ‘hydro/dehydro’ in mancude systems (see Section P-31). In some cases, especially in the case of benzene ring assemblies, assemblies of nonidentical cyclic systems result from such operations.

P-29 PREFIXES DENOTING SUBSTITUENT GROUPS DERIVED FROM PARENT HYDRIDES

P-29.0 Introduction
P-29.1 Definitions
P-29.2 General methodology for naming substituent groups
P-29.3 Systematic names for simple substituent prefixes derived from saturated parent hydrides
P-29.4 Compound substituent groups
P-29.5 Complex substituent groups
P-29.6 Retained names for prefixes of simple substituent groups derived from the parent hydrides described in Chapter P-2

P-29.0 INTRODUCTION

This Section includes the names of substituent groups derived from the parent hydrides described in Sections P-21 through P-28 and used as prefixes in substitutive nomenclature. The methodology for forming systematic prefixes is fully described in this Section; preferred IUPAC prefixes are identified, as well as preselected prefixes.

P-29.1 DEFINITIONS

Substituent groups derived from parent hydrides are used in many ways in the nomenclature of organic compounds and may be classified as simple substituent groups, compound substituent groups, and complex substituent groups.

The definitions for substituent groups derived from parent hydrides given below differ from those that were previously recommended (see A-2.3 in ref. 1 and R-4.1 in ref. 2).

P-29.1.1 A simple substituent group is an atom or group of atoms considered as a unit with one or more free valences. The methodology for naming such groups is described in P-29.2. The basic multiplicative prefixes ‘di’, ‘tri’, ‘tetra’, etc. denote the presence of more than one identical simple substituent group in a compound or complex substituent group, but see P-29.1.2 and P-29.1.3 for use of derived multiplicative prefixes, such as ‘bis’, ‘tris’, ‘tetrakis’.

P-29.1.2 A compound substituent group consists of a simple substituent group (the parent substituent group) to which is attached one or more simple substituent groups. Compound substituent group names are formed by combining the names of two or more simple substituent groups. There are three ways to accomplish this:

(1) by the substitutive operation;

(2) by an additive operation;

(3) by combined substitutive and additive operations.

Compound substituent groups are formed by the substitution operation rather than by an additive operation unless the simple parent substituent group is not acceptable for substitution, i.e., it has no substitutable hydrogen atoms. Compound substituent groups formed by substitution are cited in names as prefixes, often called ‘substituent prefixes’. Compound substituent groups formed by addition are cited in names as prefixes, often called ‘concatenated prefixes’. The derived multiplicative prefixes ‘bis’, ‘tris’, ‘tetrakis’, etc. are used to multiply compound prefixes and to avoid ambiguity when the basic multiplying prefixes are already part of the name of a substituent group (see P-16.3).

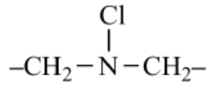
Examples:

$-CH_2\text{-}Cl$
chloromethyl (preferred prefix)
(a substitutive prefix; see P-13.1)

$-CO\text{-}Cl$
carbonochloridoyl (preferred prefix)
(a concatenated prefix; see P-13.3.4)

Mixed concatenated substituent groups are formed by substitution to introduce substituent groups into one or more of their components.

Example:

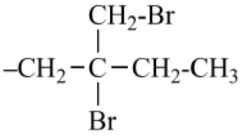


$-CH_2-\overset{\overset{\text{Cl}}{|}}{N}-CH_2-$

(chloroazanediyl)bis(methylene) (preferred prefix)

P-29.1.3 A complex substituent group consists of a parent substituent group to which is attached, by substitution or concatenation, at least one compound substituent group. In a complex substituent group, the parent substituent group of a component compound substituent group is called a subsidiary parent substituent group. Multiplicative prefixes, used as the central part in multiplicative nomenclature (see P-15.3.2), are formed by the additive operation, and when these consist of three or more parts are considered as ‘complex concatenated prefixes’. The derived multiplicative prefixes ‘bis’, ‘tris’, ‘tetrakis’, etc. are used to multiply complex prefixes and to avoid ambiguity when the basic multiplying prefixes are already part of the name of a substituent group (see P-16.3).

Examples:



$-CH_2-\underset{\underset{\text{Br}}{|}}{\overset{\overset{CH_2\text{-}Br}{|}}{C}}-CH_2\text{-}CH_3$

2-bromo-2-(bromomethyl)butyl (preferred prefix: a complex substituted prefix)

$>N\text{-}CH_2\text{-}O\text{-}CH_2\text{-}N<$
oxybis(methylenenitrilo) (preferred prefix; a complex concatenated prefix)

Concatenation and substitution can be combined to form substituted concatenated complex substituent groups.

Example:

$-CHCl\text{-}O\text{-}CH_2\text{-}CH_2\text{-}O\text{-}CHCl-$
ethane-1,2-diylbis[oxy(chloromethylene)] (preferred prefix)

P-29.2 GENERAL METHODOLOGY FOR NAMING SUBSTITUENT GROUPS

The presence of free valences formally derived from the loss of one or more hydrogen atoms from a parent hydride is denoted by suffixes ‘yl’, ‘ylidene’, and ‘ylidyne’, together with multiplying prefixes indicating the number of free valences; lowest locants are assigned to all free valences as a set, then in the order ‘yl’, ‘ylidene’, ‘ylidyne’. In names, the suffixes are cited in the order ‘yl’, ‘ylidene’, ‘ylidyne’. The suffixes ‘ylidene’ and ‘ylidyne’ are used only to indicate the attachment of a substituent to a parent hydride or parent substituent by a double or triple bond, respectively.

Monovalent	Divalent	Trivalent	Tetravalent, etc.
-yl	-diyl	-triyl	-tetrayl, etc.
	-ylidene	-ylidyne	-ylylidyne, etc.
		-ylylidene	-diylidene, etc.
			-diylylidene , etc.

Systematic names are formed by using the suffixes ‘yl’, ‘ylidene’ and ‘ylidyne’, with elision of the final letter ‘e’ of parent hydrides, when present, according to two methods:

(1) The suffixes ‘yl’, ‘ylidene’, and ‘ylidyne’ replace the ending ‘ane’ of the parent hydride name. The atom with the free valence terminates a chain and always has the locant ‘1’, which is omitted from the name. This method is recommended primarily for saturated acyclic and monocyclic hydrocarbon substituent groups and for the mononuclear hydrides of silicon, germanium, tin, and lead. Substituent groups formed by this method are referred to as ‘alkyl-type substituent groups’;

(2) The suffixes ‘yl’, ‘ylidene’, and ‘ylidyne’ are added to the name of the parent hydride with elision of the terminal letter ‘e’, if present, when followed immediately by the letter ‘y’. The locants for the atoms of free valences are as low as is consistent with any established numbering of the parent hydride and, except for mononuclear parent hydrides or the suffix ‘ylidyne’, the locant ‘1’ must be cited. This method is used to generate names of ‘alkanyl-type substituent groups’ that are simple substituent groups with free valences at positions other than ‘1’.

Method (1) is no longer applicable to boron prefixes.

For the application of these methods in generating preferred IUPAC names, see P-57.1.1.1.

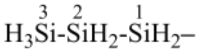
Examples:

$CH_3–$
methyl (preferred prefix)
methanyl

$SiH_3–$
silyl (preselected prefix)

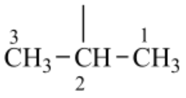
$CH_2=$
methylidene (preferred prefix)
methanylidene

$CH_3 C≡$
ethylidyne (preferred prefix)
ethanylidyne



$$\overset{3}{H_3Si}\text{-}\overset{2}{SiH_2}\text{-}\overset{1}{SiH_2}–$$

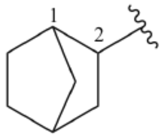
trisilan-1-yl (preselected prefix)



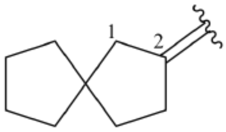
$$\overset{3}{CH_3}-\underset{2}{\overset{|}{CH}}-\overset{1}{CH_3}$$

propan-2-yl (preferred prefix)
1-methylethyl

$C_6H_{11}–$
cyclohexyl (preferred prefix)



bicyclo[2.2.1]heptan-2-yl (preferred prefix)
bicyclo[2.2.1]hept-2-yl



spiro[4.4]nonan-2-ylidene (preferred prefix)
spiro[4.4]non-2-ylidene

P-29.3 SYSTEMATIC NAMES FOR SIMPLE SUBSTITUENT PREFIXES DERIVED FROM SATURATED PARENT HYDRIDES

P-29.3.1 Substituent prefixes derived from mononuclear parent hydrides
P-29.3.2 Substituent prefixes derived from acyclic parent hydrides

P-29.3.3 Substituent prefixes derived from saturated cyclic parent hydrides
P-29.3.4 Substituent prefixes derived from mancude parent hydrides
P-29.3.5 Substituent prefixes derived from ring assemblies
P-29.3.6 Substituent prefixes derived from phane systems

P-29.3.1 Substituent prefixes derived from mononuclear parent hydrides

Simple substituent groups derived from the mononuclear parent hydrides of carbon, silicon, germanium, tin, and lead (boron is no longer included) traditionally have been named by method (1) in P-29.2. Other mononuclear parent hydrides, i.e., those derived from O, F, Cl, Br, I, S, Se, Te, N, P, As, Sb, Bi, B, Al, Ga, In, and Tl, are named by method (2) in P-29.2. The prefix 'amino' is retained as the preselected prefix for $-NH_2$, and the prefixes phosphino, arsino, and stibino may be used in general nomenclature. Substituent groups derived from mononuclear parent hydrides modified by the λ-convention are discussed in P-68.3.2 for elements of Group 15, in P-68.4.3 for elements of Group 16, and in P-68.5.1 for elements of Group 17.

Prefixes derived from borane are now named only by method (2) in P-29.2, for example 'boranyl', 'boranylidene', and 'boranylidyne'.

Examples:

CH_3-
methyl (preferred prefix)
methanyl [see P-29.2 (2)]

GeH_3-
germyl (preselected prefix)

BH_2-
boranyl (preselected prefix)
(not boryl)

$CH_2=$
methylidene (preferred prefix)
methanylidene [see P-29.2 (2)]

$SnH_2=$
stannylidene (preselected prefix)

$BH=$
boranylidene (preselected prefix)
(not borylidene)

$HS-$
sulfanyl (preselected prefix)
(no longer mercapto)

H_2P-
phosphanyl (preselected prefix)
phosphino

$HAs=$
arsanylidene (preselected prefix)
(not arsinidine)

H_2Al-
alumanyl (preselected prefix)

$HAl=$
alumanylidene (preselected prefix)

$S=$
sulfanylidene (preselected prefix)
thioxo

$HSi\equiv$
silylidyne (preselected prefix)

$P\equiv$
phosphanylidyne (preselected prefix)
(not phosphinidyne)

P-29.3.2 Substituent prefixes derived from acyclic parent hydrides

Names for simple substituent groups derived from names of acyclic parent hydrides are formed by both methods described in P-29.2.

P-29.3.2.1 Names for simple substituent groups derived from acyclic hydrocarbons with a single free valence at the end of the longest chain are traditionally formed according to method (1) of P-29.2. They are generically called ‘alkyl’, ‘alkylidene’, and ‘alkylidyne’ substituent groups. The free valences are assigned the locant 1, which is omitted in names.

Examples:

$\overset{2}{C}H_3\text{-}\overset{1}{C}H_2\text{–}$
ethyl (preferred prefix)

$\overset{3}{C}H_3\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}H_2\text{–}$
propyl (preferred prefix)

$CH_3\text{-}\overset{3}{C}H_2\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}H_2\text{–}$
butyl (preferred prefix)

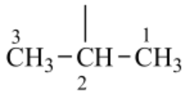
$\overset{3}{C}H_3\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}H\text{=}$
propylidene (preferred prefix)

$\overset{4}{C}H_3\text{-}\overset{3}{C}H_2\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}\equiv$
butylidyne (preferred prefix)

P-29.3.2.2 Names for simple substituent groups other than those described in P-29.3.2.1 are formed according to method (2) of P-29.2 For hydrocarbon groups, these substituent groups are generically called ‘alkanyl’, ‘alkanylidene’, ‘alkanylidyne’, ‘alkanediyl’, ‘alkanylylidene’, etc. substituent groups Low locants are assigned to free valences considered as a set, in accordance with the numbering of the chain. If there is a choice, low locants are assigned, in order, to the suffixes ‘yl’, ‘ylidene’, and ‘ylidyne’. In names, the suffixes are cited in the order ‘yl’, ‘ylidene’, and ‘ylidyne’.

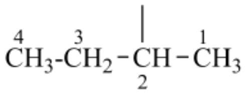
Examples:

$\overset{3}{C}H_3\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}H_2\text{–}$
propan-1-yl
propyl (preferred prefix)



$\overset{3}{C}H_3-\underset{2}{\overset{|}{C}}H-\overset{1}{C}H_3$

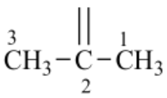
propan-2-yl (preferred prefix)
(not prop-2-yl)



$\overset{4}{C}H_3\text{-}\overset{3}{C}H_2-\underset{2}{\overset{|}{C}}H-\overset{1}{C}H_3$

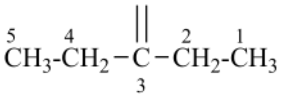
butan-2-yl (preferred prefix)
(not but-2-yl)

$\overset{4}{C}H_3\text{-}\overset{3}{C}H_2\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}\equiv$
butanylidyne
butylidyne (preferred prefix)



$\overset{3}{C}H_3-\underset{2}{\overset{||}{C}}-\overset{1}{C}H_3$

propan-2-ylidene (preferred prefix)



$$\overset{5}{C}H_3\text{-}\overset{4}{C}H_2-\underset{3}{\overset{\|}{C}}-\overset{2}{C}H_2\text{-}\overset{1}{C}H_3$$

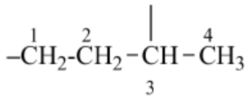
pentan-3-ylidene (preferred prefix)

$$-\overset{3}{C}H_2\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}H_2-$$

propane-1,3-diyl (preferred prefix)
(not trimethylene)

$$\overset{2}{C}H_3\text{-}\overset{1}{C}H<$$

ethane-1,1-diyl (preferred prefix)
(not ethylidene)

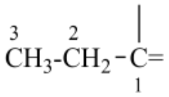


$$-\overset{1}{C}H_2\text{-}\overset{2}{C}H_2-\underset{3}{\overset{|}{C}H}-\overset{4}{C}H_3$$

butane-1,3-diyl (preferred prefix)
1-methylpropane-1,3-diyl

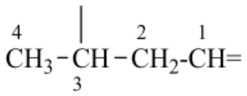
$$-\overset{1}{C}H_2\text{-}\overset{2}{C}H=$$

ethan-1-yl-2-ylidene (preferred prefix)



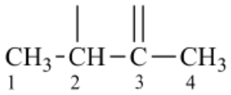
$$\overset{3}{C}H_3\text{-}\overset{2}{C}H_2-\underset{1}{\overset{|}{C}}=$$

propan-1-yl-1-ylidene (preferred prefix)



$$\overset{4}{C}H_3-\underset{3}{\overset{|}{C}H}-\overset{2}{C}H_2\text{-}\overset{1}{C}H=$$

butan-3-yl-1-ylidene (preferred prefix)



$$\underset{1}{CH_3}-\underset{2}{\overset{|}{CH}}-\underset{3}{\overset{\|}{C}}-\underset{4}{CH_3}$$

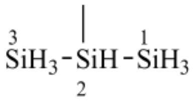
butan-2-yl-3-ylidene (preferred prefix)

$AsH_2\text{-}AsH-$
diarsanyl (preselected prefix)

$SiH_3\text{-}SiH_2-$
disilanyl (preselected prefix)

$$\overset{3}{N}H_2\text{-}\overset{2}{N}H\text{-}\overset{1}{N}H-$$

triazan-1-yl (preselected prefix)



$$\overset{3}{Si}H_3-\underset{2}{\overset{|}{SiH}}-\overset{1}{Si}H_3$$

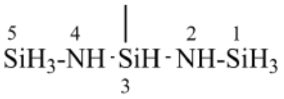
trisilan-2-yl (preselected prefix)

$$\overset{3}{Si}H_3\text{-}\overset{2}{O}\text{-}\overset{1}{Si}H_2-$$

disiloxanyl (preselected prefix)

$SiH_3\text{-}NH\text{-}SiH_2-$
(silylamino)silyl (preselected prefix)
(not disilazan-1-yl;
disilazane is not a recommended parent, hydride,see P-21.2.3.1)

$(SiH_3)_2N-$
disilylamino (preselected prefix)
(not disilazan-2-yl;
disilazane is not a recommended parent hydride, see P-21.2.3.1)



$\overset{5}{SiH_3}\text{-}\overset{4}{NH}\text{-}\underset{3}{\overset{|}{SiH}}\text{-}\overset{2}{NH}\text{-}\overset{1}{SiH_3}$

bis(silylamino)silyl (preselected prefix)
(not trisilazan-3-yl;
trisilazane is not a recommended parent hydride, see P-21.2.3.1)

$H_2N\text{-}NH\text{–}$
hydrazinyl (preselected prefix)
diazanyl

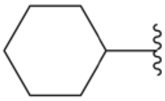
$H_2N\text{-}N\text{=}$
hydrazinylidene (preselected prefix)
diazanylidene

$\overset{1}{CH_3}\text{-}\overset{2}{O}\text{-}\overset{3}{CH_2}\text{-}\overset{4}{CH_2}\text{-}\overset{5}{O}\text{-}\overset{6}{CH_2}\text{-}\overset{7}{CH_2}\text{-}\overset{8}{O}\text{-}\overset{9}{CH_2}\text{-}\overset{10}{CH_2}\text{-}\overset{11}{O}\text{-}\overset{12}{CH_2}\text{-}\overset{13}{CH_2}\text{-}\overset{14}{CH_2}\text{–}$
2,5,8,11-tetraoxatetradecan-14-yl (preferred prefix)

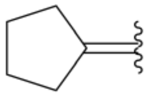
P-29.3.3 Substituent prefixes derived from saturated cyclic parent hydrides

Names for monovalent substituent groups derived from cycloalkanes are formed traditionally by method (1) in P-29.2. Names for all other substituent groups derived from saturated cyclic parent hydrides are named by method (2) in P-29.2. Low locants are assigned to free valences 'yl', 'ylidene', and 'ylidyne' in accordance with the numbering of the parent hydride. If there is a choice, the suffixes are assigned low locants, in that order. Suffixes are cited in the order 'yl', 'ylidene', and 'ylidyne'. For preferred names see P-57.1.5.1.

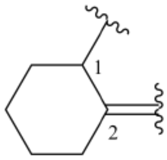
Examples:



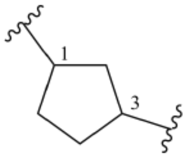
cyclohexyl (preferred prefix)
cyclohexanyl



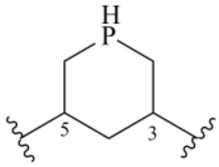
cyclopentylidene (preferred prefix)
cyclopentanylidene



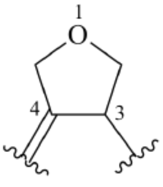
cyclohexan-1-yl-2-ylidene (preferred prefix)



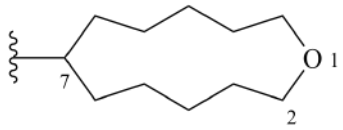
cyclopentane-1,3-diyl (preferred prefix)



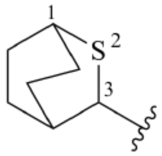
phosphinane-3,5-diyl (preferred prefix)



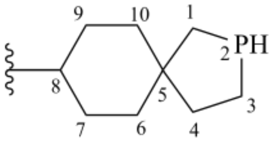
oxolan-3-yl-4-ylidene (preferred prefix)



1-oxacyclododecan-7-yl (preferred prefix)



2-thiabicyclo[2.2.2]octan-3-yl (preferred prefix)

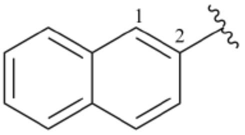


2-phosphaspiro[4.5]decan-8-yl (preferred prefix)

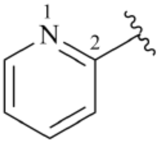
P-29.3.4 Substituent prefixes derived from mancude parent hydrides

P-29.3.4.1 All mancude rings and ring systems are named by method (2) in P-29.2. When one hydrogen atom is present, there is no difficulty in deriving a monovalent substituent. When no hydrogen atoms are present or when an 'ylidene' type substituent group is needed, it is necessary to use 'added indicated hydrogen' (see P-14.7). Formally, this method involves the adding of one hydrogen atom to the atom from which the substituent group is derived and another hydrogen atom that can be located on any atom of the ring or ring system. This 'added indicated hydrogen atom' is expressed by the symbol *H*, preceded by a locant denoting its position.

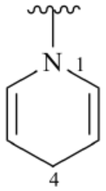
Examples:



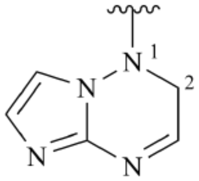
naphthalen-2-yl (preferred prefix)



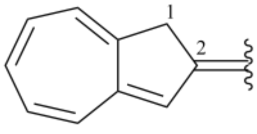
pyridin-2-yl (preferred prefix)



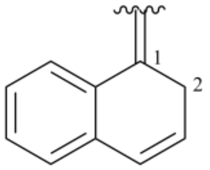
pyridin-1(4*H*)-yl (preferred prefix)



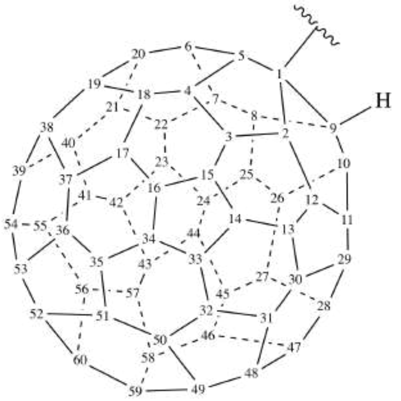
imidazo[1,2-*b*][1,2,4]triazin-1(2*H*)-yl (preferred prefix)



azulen-2(1*H*)-ylidene (preferred prefix)



naphthalen-1(2*H*)-ylidene (preferred prefix)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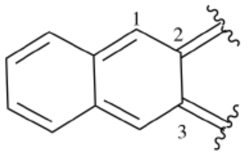
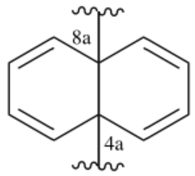
(C_{60}-I_h)[5,6]fulleren-1(9*H*)-yl (preferred prefix)

P-29.3.4.2 ‘Diylidene’ substituent groups derived from mancude compounds by conversion of two H atoms into free valences with any necessary rearrangement of double bonds to a quinoid structure are named by adding two ‘ylidene’ suffixes, that is ‘diylidene’, to the parent hydride; no added hydrogen is necessary. Also, no added hydrogen is necessary in the case of the formation of a ‘diyl’ substituent group when the free valences are located at fusion atoms.

Examples:



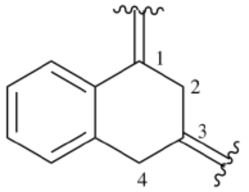
naphthalene-2,3-diylidene (preferred prefix)



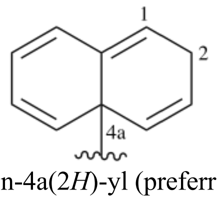
naphthalene-4a,8a-diyl (preferred prefix)

When no quinoid structure results from the introduction of free valences, added hydrogen atoms must be cited in names. They receive the lowest possible locants. When one free valence of the ‘yl’ type is present at a fusion atom, added hydrogen must also be cited in names.

Examples:



naphthalene-1,3(2*H*,4*H*)-diylidene (preferred prefix)



naphthalen-4a(2*H*)-yl (preferred prefix)

P-29.3.5 Substituent prefixes derived from ring assemblies

Names of ring assemblies composed of two identical rings or ring systems are formed as described in Section P-28.2, and those derived from ring assemblies composed of three through six identical rings or ring systems are described in

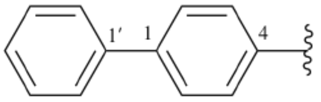
P-28.3. Ring assemblies consisting of more than six rings or ring assemblies are named by phane nomenclature as described in P-28.5. Low locants are assigned to ring junctions, then to free valences.

Names of substituent groups derived from ring assemblies are written in two ways:

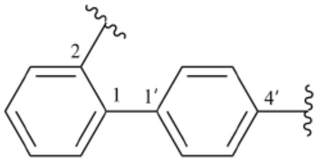
(1) the suffix ‘yl’ is added to the name biphenyl;

(2) names denoted by locants are placed in brackets; the suffixes ‘yl’ and ‘ylidene’ are added with elision of the final letter ‘e’ in the name of the parent hydride.

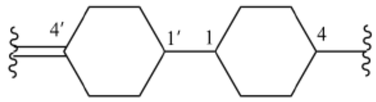
Examples:



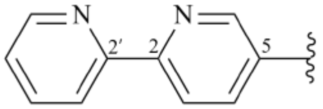
[1,1′-biphenyl]-4-yl (preferred prefix)



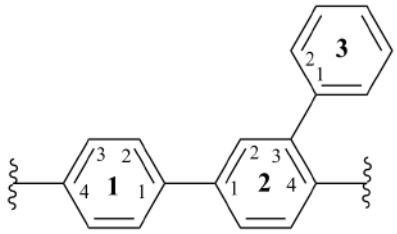
[1,1′-biphenyl]-2,4′-diyl (preferred prefix)



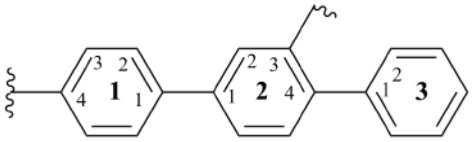
[1,1′-bi(cyclohexan)]-4-yl-4′-ylidene (preferred prefix)
[1,1′-bi(cyclohexyl)]-4-yl-4′-ylidene



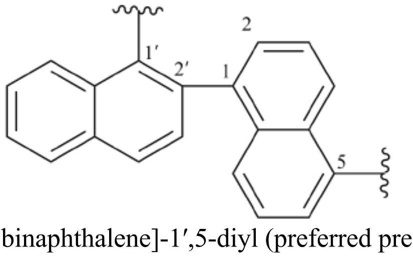
[2,2′-bipyridin]-5-yl (preferred prefix)
[2,2′-bipyridyl]-5-yl



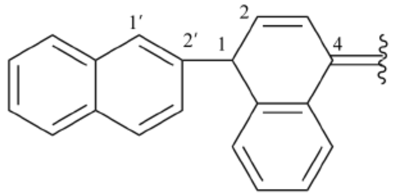
[1^1,2^1:2^3,3^1-terphenyl]-1^4,2^4-diyl (preferred prefix)
[1,1′:3′,1″-terphenyl]-4,4′-diyl



[1^1,2^1:2^4,3^1-terphenyl]-1^4,2^3-diyl (preferred prefix)
[1,1′:4′,1″-terphenyl]-3′,4-diyl



[1,2′-binaphthalene]-1′,5-diyl (preferred prefix)
[1,2′-binaphthyl]-1′,5-diyl

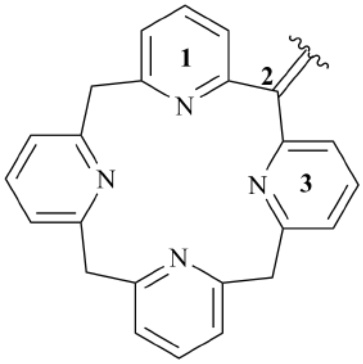


[1,2′-binaphthalen]-4(1*H*)-ylidene (preferred prefix)
1,2′-binaphthyl]-4(1*H*)-ylidene

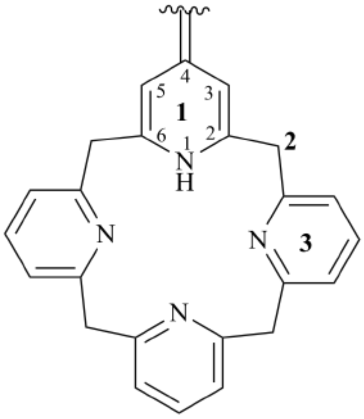
P-29.3.6 Substituent prefixes derived from phane systems

Substituent groups derived from cyclophanes are formed by applying the principles described above.

Examples:



1,3,5,7(2,6)-tetrapyridinacyclooctaphan-2-ylidene (preferred prefix)



1,3,5,7(2,6)-tetrapyridinacyclooctaphan-$1^4(1^1H)$-ylidene (preferred prefix)

P-29.4 COMPOUND SUBSTITUENT GROUPS

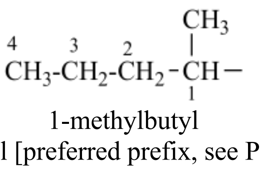
P-29.4.1 Compound substituted substituent groups

A compound substituted substituent group is formed by substituting one or more simple substituents into another simple substituent that is considered as the principal chain. The choice of the principal chain is fully discussed in Section P-44.3. The first criterion to be applied is that the principal chain is the longest chain; it will be applied in the following examples of acyclic compound substituent groups.

Mono-, di-, and polyvalent substituent groups derived from homogeneous chains are named by prefixing the designation of the side chains to the name of the unbranched substituent group possessing the longest possible chain. When a choice is possible, lowest locants are assigned to the side chain. The presence of identical simple substituent groups is indicated by the appropriate multiplying prefix ‘di’, ‘tri’, ‘tetra’, etc.

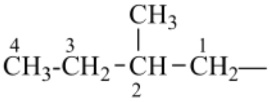
Names of substituent groups are formed in accordance with P-29.3. Substituent groups of compound substitutive groups must be named by the preferred IUPAC name, as described in Chapter P-5, or preselected name.

Examples:



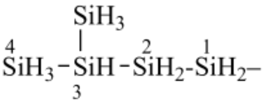
$$\overset{4}{CH_3}\text{-}\overset{3}{CH_2}\text{-}\overset{2}{CH_2}\text{-}\underset{1}{\overset{\overset{CH_3}{|}}{CH}}-$$

1-methylbutyl
pentan-2-yl [preferred prefix, see P-29.2 (2)]



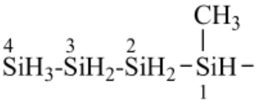
$$\overset{4}{\mathrm{C}}\mathrm{H_3}\text{-}\overset{3}{\mathrm{C}}\mathrm{H_2}\text{-}\underset{2}{\overset{\overset{\mathrm{CH_3}}{|}}{\mathrm{C}}}\mathrm{H}-\overset{1}{\mathrm{C}}\mathrm{H_2}\text{—}$$

2-methylbutyl (preferred prefix)



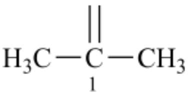
$$\overset{4}{\mathrm{Si}}\mathrm{H_3}-\underset{3}{\overset{\overset{\mathrm{SiH_3}}{|}}{\mathrm{Si}}}\mathrm{H}-\overset{2}{\mathrm{Si}}\mathrm{H_2}\text{-}\overset{1}{\mathrm{Si}}\mathrm{H_2}\text{–}$$

3-silyltetrasilan-1-yl (preselected prefix)



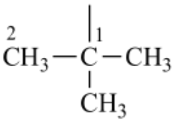
$$\overset{4}{\mathrm{Si}}\mathrm{H_3}\text{-}\overset{3}{\mathrm{Si}}\mathrm{H_2}\text{-}\overset{2}{\mathrm{Si}}\mathrm{H_2}-\underset{1}{\overset{\overset{\mathrm{CH_3}}{|}}{\mathrm{Si}}}\mathrm{H}-$$

1-methyltetrasilan-1-yl (preferred prefix)



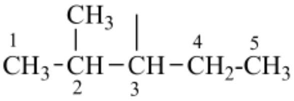
$$\mathrm{H_3C}-\underset{1}{\overset{||}{\mathrm{C}}}-\mathrm{CH_3}$$

1-methylethylidene
propan-2-ylidene (preferred prefix)



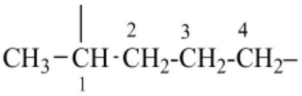
$$\overset{2}{\mathrm{C}}\mathrm{H_3}-\underset{\underset{\mathrm{CH_3}}{|}}{\overset{|\,1}{\mathrm{C}}}-\mathrm{CH_3}$$

1,1-dimethylethyl (numbering shown)
2-methylpropan-2-yl
tert-butyl (preferred prefix, see P-29.6)



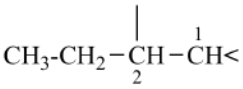
$$\overset{1}{\mathrm{C}}\mathrm{H_3}\text{-}\underset{2}{\overset{\overset{\mathrm{CH_3}}{|}}{\mathrm{C}}}\mathrm{H}-\underset{3}{\overset{|}{\mathrm{C}}}\mathrm{H}-\overset{4}{\mathrm{C}}\mathrm{H_2}\text{-}\overset{5}{\mathrm{C}}\mathrm{H_3}$$

2-methylpentan-3-yl (preferred prefix)
(not 4-methylpentan-3-yl;
locant ‘2’ is lower than ‘4’)



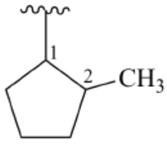
$$\mathrm{CH_3}-\underset{1}{\overset{|}{\mathrm{C}}}\mathrm{H}\cdot\overset{2}{\mathrm{C}}\mathrm{H_2}\text{-}\overset{3}{\mathrm{C}}\mathrm{H_2}\text{-}\overset{4}{\mathrm{C}}\mathrm{H_2}\text{–}$$

1-methylbutane-1,4-diyl
pentane-1,4-diyl (preferred prefix)

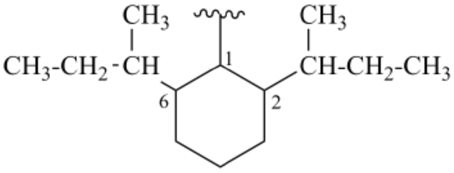


$$\mathrm{CH_3}\text{-}\mathrm{CH_2}-\underset{2}{\overset{|}{\mathrm{C}}}\mathrm{H}-\overset{1}{\mathrm{C}}\mathrm{H}<$$

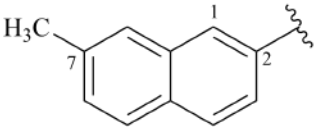
2-ethylethane-1,1,2-triyl
butane-1,1,2-triyl (preferred prefix)



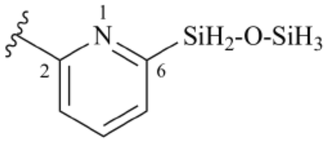
2-methylcyclopentyl (preferred prefix)



2,6-di(butan-2-yl)cyclohexyl (preferred prefix)



7-methylnaphthalen-2-yl (preferred prefix)



6-disiloxanylpyridin-2-yl (preferred prefix)

P-29.4.2 Compound catenated substituent groups

Compound catenated substituent groups are used only in multiplicative nomenclature (see P-15.3). Names are formed by adding di- or polyvalent substituent groups to one another, specifically by adding the names of peripheral substituent groups to that of a central substituent group, as prescribed in multiplicative nomenclature (see P-15.3). Substitution of components is allowed when the symmetry of the whole substituent group is preserved.

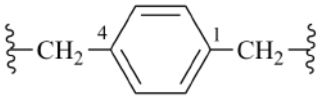
Examples:

$$-CH_2\text{-}CH_2\text{-}SiH_2\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}H_2-$$

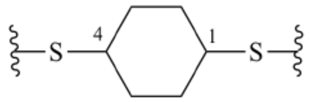
silanediyldi(ethane-2,1-diyl) (preferred prefix)
silanediyldiethylene

$$-SiH_2\text{-}SiH_2\text{-}CH_2\text{-}\overset{2}{Si}H_2\text{-}\overset{1}{Si}H_2-$$

methylenebis(disilane-2,1-diyl) (preferred prefix)



1,4-phenylenebis(methylene) (preferred prefix;
1,4-phenylene and methylene are preferred retained IUPAC prefixes, see P-29.6.1)



cyclohexane-1,4-diylbis(sulfanediyl) (preferred prefix)
cyclohexane-1,4-diylbis(thio)

$$-CHF\text{-}CH_2\text{-}SiH_2\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}HF-$$

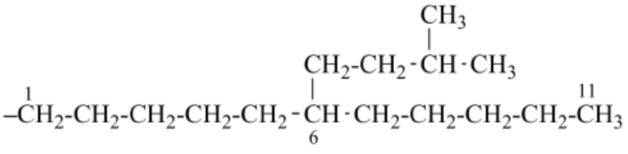
silanediylbis(1-fluoroethane-2,1-diyl) (preferred prefix)
[not silanediylbis(1-fluoroethylene)]

P-29.5 COMPLEX SUBSTITUENT GROUPS

P-29.5.1 Complex substituted substituent groups

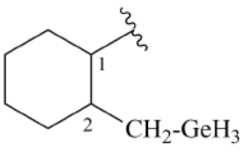
Complex substituted substituent groups are formed by substituting an acyclic compound substitutive substituent group into an acyclic substituent group, or into a cyclic substituent group, in accordance with the order of seniority of chains and rings and ring systems (P-44).

Examples:



$$-\overset{1}{C}H_2\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}\underset{6}{\overset{\overset{\displaystyle CH_3}{|}}{\overset{CH_2\text{-}CH_2\text{-}CH\text{-}CH_3}{\overset{|}{C}}}}H\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}\overset{11}{C}H_3$$

6-(3-methylbutyl)undecyl (preferred prefix)



2-(germylmethyl)cyclohexyl (preferred prefix)

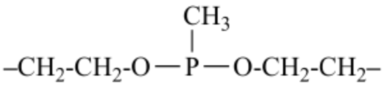
P-29.5.2 Concatenated complex substituent groups

Concatenated substituent groups are complex substituent groups when they are composed of three or more components. Substitution is allowed as long as the symmetry of the group is maintained.

Examples:

$–O-CH_2-S-CH_2-O–$

sulfanediylbis(methyleneoxy) (preferred prefix)



$$–CH_2-CH_2-O—\overset{\overset{CH_3}{|}}{P}—O-CH_2-CH_2–$$

(methylphosphanediyl)bis(oxyethane-2,1-diyl) (preferred prefix)

P-29.6 RETAINED NAMES FOR PREFIXES OF SIMPLE SUBSTITUENT GROUPS DERIVED FROM THE PARENT HYDRIDES DESCRIBED IN CHAPTER P-2

Three aspects of the use in nomenclature of simple substituent groups derived from parent hydrides with retained names are discussed in this Section:

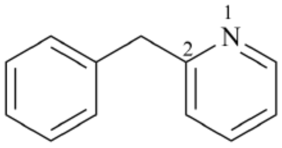
P-29.6.1 Retained prefixes that are preferred prefixes;
P-29.6.2 Retained prefixes that are not used as preferred prefixes;
P-29.6.3 Retained prefixes no longer recommended as approved prefixes.

P-29.6.1 Retained prefixes that are preferred prefixes

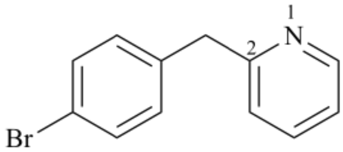
The traditional prefixes benzyl, benzylidene, benzylidyne are retained preferred prefixes, but are not to be substituted; however, see P-29.6.2.

> In the 1993 Guide (ref. 2), the names ‘benzyl’, ‘benzylidene’, and ‘benzylidyne’ could only be substituted on the ring. In these recommendations, however, for preferred prefixes substitution is not allowed on the ring nor on the side chain, but for general nomenclature, restricted substitution is permitted (see P-29.6.2).

Examples:



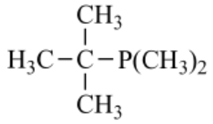
2-benzylpyridine (PIN)
2-(phenylmethyl)pyridine



2-(4-bromobenzyl)pyridine
2-[(4-bromophenyl)methyl]pyridine (PIN)

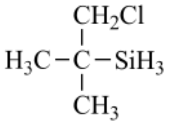
The retained name ‘*tert*-butyl’ has never been recommended for further substitution; this is maintained in these recommendations. Acceptable locants have never been adopted for this name. The names ‘methanediyl’ and ‘benzene-1,2-diyl’ are not recommended in place of ‘methylene’ and ‘1,2-phenylene’, respectively. The names ‘trimethylene’, ‘tetramethylene’, etc. are not recommended.

Examples:



$$H_3C-\underset{\underset{CH_3}{|}}{\overset{\overset{CH_3}{|}}{C}}-P(CH_3)_2$$

tert-butyldi(methyl)phosphane (PIN)
(1,1-dimethylethyl)di(methyl)phosphane



$$H_3C-\underset{\underset{CH_3}{|}}{\overset{\overset{CH_2Cl}{|}}{C}}-SiH_3$$

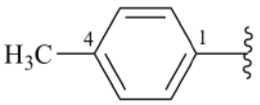
(1-chloro-2-methylpropan-2-yl)silane (PIN)
(2-chloro-1,1-dimethylethyl)silane

The retained prefixes ‘methylene’, ‘phenyl’, and ‘1,2-, 1,3-, and 1,4-phenylene’ have been used as fully substitutable substituent groups; this is maintained in these recommendations for simple, compound, and complex substituent groups.

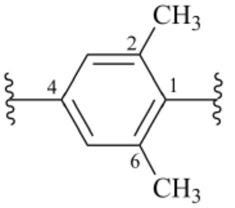
Examples:

–CHBr–

bromomethylene (preferred prefix)



4-methylphenyl (preferred prefix)



2,6-dimethyl-1,4-phenylene (preferred prefix)

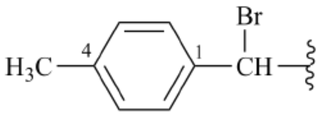
P-29.6.2 Retained prefixes that are not used as preferred prefixes

P-29.6.2.1 The prefixes benzyl, benzylidene, and benzylidyne are preferred prefixes when unsubstituted. However, these prefixes may be used in general nomenclature when substituted as follows:

(1) unlimited ring substitution;

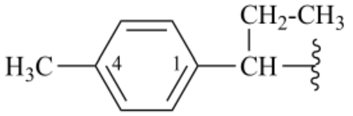
(2) substitution on the α-position by characteristic atoms or groups that are compulsory substituents (see Table 5.1) or by substituent groups that do not extend the chain.

Examples:



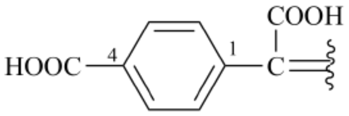
bromo(4-methylphenyl)methyl (preferred prefix)

α-bromo-4-methylbenzyl



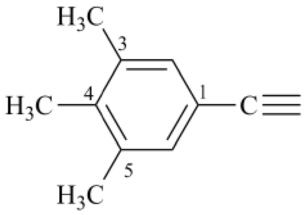
1-(4-methylphenyl)propyl (preferred prefix)

(not α-ethyl-4-methylbenzyl)



α,4-dicarboxybenzylidene

carboxy(4-carboxyphenyl)methylidene (preferred prefix)

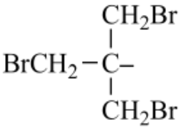


3,4,5-trimethylbenzylidyne

(3,4,5-trimethylphenyl)methylidyne (preferred prefix)

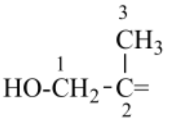
P-29.6.2.2 The prefixes isopropyl, isopropylidene, and trityl are retained for use in general nomenclature but no substitution of any kind is allowed.

Examples:



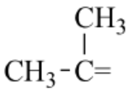
$$BrCH_2-\overset{\displaystyle CH_2Br}{\underset{\displaystyle CH_2Br}{\overset{|}{\underset{|}{C}}}}-$$

1,3-dibromo-2-(bromomethyl)propan-2-yl (preferred prefix)
2-bromo-1,1-bis(bromomethyl)ethyl



$$\overset{1}{HO}\text{-}CH_2\text{-}\overset{\overset{3}{CH_3}}{\underset{2}{C}}=$$

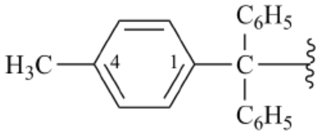
1-hydroxypropan-2-ylidene (preferred prefix)
2-hydroxy-1-methylethylidene



$$CH_3\text{-}\overset{CH_3}{C}=$$

propan-2-ylidene (preferred prefix)
1-methylethylidene
isopropylidene (no substitution allowed)

$(C_6H_5)_3C$–
trityl (no substitution allowed)
triphenylmethyl (preferred prefix)



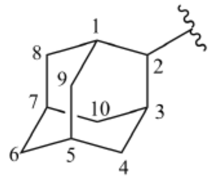
(4-methylphenyl)di(phenyl)methyl (preferred prefix)

P-29.6.2.3 The prefix ethylene and the following traditional prefixes for ring substituents are retained but only for general nomenclature and are fully substitutable.

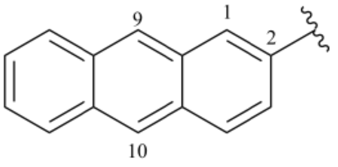
Examples:

$–CH_2\text{-}CH_2–$
ethylene
ethane-1,2-diyl (preferred prefix)

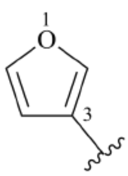
–CHCl-CHCl–
1,2-dichloroethylene
1,2-dichloroethane-1,2-diyl (preferred prefix)



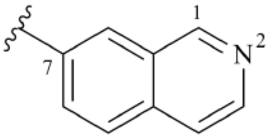
2-adamantyl (also 1-isomer)
adamantan-2-yl (preferred prefix)
tricyclo[3.3.1.1^{3,7}]decan-2-yl



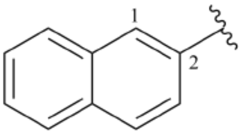
2-anthryl (also 1- and 9-isomers)
anthracen-2-yl (preferred prefix)



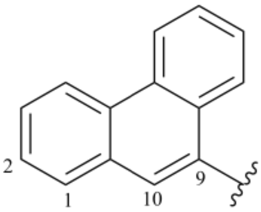
3-furyl (also 2-isomer)
furan-3-yl (also 2-isomer; preferred prefixes)



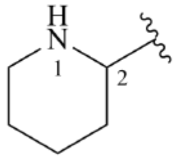
7-isoquinolyl (also 1-, 3-, 4-, 5-, 6- and 8-isomers)
isoquinolin-7-yl (also 1-, 3-, 4-, 5-, 6- and 8-isomers; preferred prefixes)



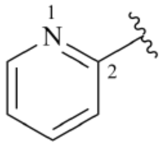
2-naphthyl (also 1-isomer)
naphthalen-2-yl (also 1-isomer; preferred prefixes)



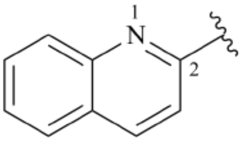
9-phenanthryl (also 1-, 2-, 3- and 4-isomers)
phenanthren-9-yl (also 1-, 2-, 3- and 4-isomers; preferred prefixes)



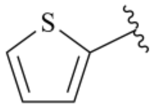
2-piperidyl (also 1-, 3- and 4-isomers)
piperidin-2-yl (also 1-, 3- and 4-isomers; preferred prefixes)



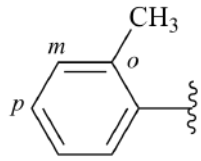
2-pyridyl (also 3- and 4-isomers)
pyridin-2-yl (also 3- and 4-isomers; preferred prefixes)



2-quinolyl (also 3-, 4-, 5-, 6-, 7- and 8-isomers)
quinolin-2-yl (also 3-, 4-, 5-, 6-, 7- and 8-isomers; preferred prefixes)



2-thienyl (also 3-isomer)
thiophen-2-yl (also 3-isomer; preferred prefixes)



o-tolyl (also *m*- and *p*-isomers; no substitution allowed)
2-methylphenyl (also 3- and 4-isomers; preferred prefixes)

P-29.6.3 Retained prefixes no longer recommended as approved prefixes

Trivial, common, and traditional prefixes have always been an integral part of organic nomenclature. However, as systematic nomenclature develops and becomes widely used, many of these prefixes fall by the wayside. Accordingly, each set of IUPAC recommendations contains fewer of these traditional prefixes. These recommendations are no different. The following prefixes were still contained in the 1993 recommendations (ref. 2) but are NOT recommended in these recommendations; their systematic prefixes based on these recommendations are given as ‘preferred prefixes’.

C_6H_5-CH_2-CH_2–
2-phenylethyl (preferred prefix)
(not phenethyl)

$(C_6H_5)_2CH$–
diphenylmethyl (preferred prefix)
(not benzhydryl)

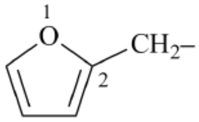
$(CH_3)_2CH$-CH_2–
2-methylpropyl (preferred prefix)
(not isobutyl)

CH_3-CH_2-$CH(CH_3)$–
butan-2-yl (preferred prefix)
1-methylpropyl
(not *sec*-butyl)

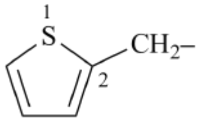
$(CH_3)_2CH$-CH_2-CH_2–
3-methylbutyl (preferred prefix)
(not isopentyl)

CH_3-CH_2-$C(CH_3)_2$–
2-methylbutan-2-yl (preferred prefix)
1,1-dimethylpropyl
(not *tert*-pentyl)

$(CH_3)_3C$-CH_2–
2,2-dimethylpropyl (preferred prefix)
(not neopentyl)



(furan-2-yl)methyl (preferred prefix)
[not furfuryl (2-isomer only)]



(thiophen-2-yl)methyl (preferred prefix)
2-thienylmethyl
[not thenyl (2-isomer only)]

International Union of Pure and Applied Chemistry

Division VIII Chemical Nomenclature and Structure Representation Division

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Chapter P-3 CHARACTERISTIC (FUNCTIONAL) AND SUBSTITUENT GROUPS

P-30 Introduction
P-31 Modification of the degree of hydrogenation of parent hydrides
P-32 Substituent prefixes for substituents derived from parent hydrides with a modified degree of hydrogenation
P-33 Suffixes
P-34 Functional parent compounds
P-35 Prefixes corresponding to characteristic groups

P-30 INTRODUCTION

The prefixes and/or suffixes attached to a parent name specify a particular molecular structure and usually represent **substituents** of various types, which are considered to take the place of hydrogen atoms of the parent hydride or parent structure. It has been customary to regard such substituents as **characteristic** (or **functional**) when the link between substituent and parent is not a carbon-carbon bond, for example, –OH, =O, and $–NH_2$, but exceptions are recognized, such as –COOH and –CN. It seems appropriate to retain the general view of **functionality** as implying the presence of heteroatoms, but it would not be helpful to attempt to define precisely the limits of application of the term.

Carbon-carbon unsaturation in acyclic and alicyclic compounds is regarded by IUPAC as a special type of functionality and is therefore treated here in Chapter P-3 rather than in Chapter P-2 (Parent Hydrides). Its presence here and that of the hydrogenation of parent hydrides having the maximum number of noncumulative double bonds (mancude parent hydrides) is logical for nomenclature, as the unsaturation in acyclic and alicyclic parent hydrides expressed by endings and the saturation of mancude parent hydrides by hydro-dehydro prefixes are essentially equivalent.

This Chapter also deals with **functional parent compounds**, i.e., structures that may be treated as parent structures, having substitutable hydrogen atoms, but possessing characteristics normally associated with functionality, e.g. acetic acid, CH_3-COOH, and phosphonic acid, $HP(O)(OH)_2$. Functional parent compounds must be distinguished from compounds having a characteristic group systematically introduced as a suffix attached to a parent hydride, for example butanoic acid and ethanol. The latter compounds may be called ‘functionalized parent hydrides’, though strictly speaking, **ions** and **radicals** do not fall within the concept of functionality as described above; an ionic center or a radical center is treated like a function and expressed in the same way as characteristic groups, i.e., by suffixes and prefixes. This treatment is introduced in this Chapter and Chapter P-7.

Any group may be expressed in a name either as a suffix or as a prefix. As prefixes, they are detachable (alphabetizable), as are the prefixes derived from parent hydrides discussed in section P-14.5.

P-31 MODIFICATION OF THE DEGREE OF HYDROGENATION OF PARENT HYDRIDES

P-31.0 Introduction
P-31.1 The endings ‘ene’ and ‘yne’
P-31.2 Substituent groups modified by the prefix ‘hydro’ and ‘dehydro’

P-31.0 INTRODUCTION

Parent hydrides are divided into two groups, fully saturated or fully unsaturated. Fully unsaturated cyclic parent hydrides are, by convention, defined as having the maximum number of noncumulative double bonds, also called ‘mancude’ compounds (an acronym for **MA**ximum number of **N**on**CU**mulated Doubl**E** bonds). Thus a degree of hydrogenation different from those denoting these two groups must be expressed by an additive or subtractive operation corresponding to the addition or the subtraction of hydrogen atoms. Specific rules are devised for compounds having saturated and unsaturated parts, such as cyclophanes, spiro compounds, etc.

The state of hydrogenation of parent hydrides is modified in two ways: (a) by a subtractive operation (subtraction of two or more hydrogen atoms) denoted by the ‘ene’ and ‘yne’ endings or by the prefix ‘dehydro’; or (b) by an additive operation (addition of two or more hydrogen atoms) denoted by the prefix ‘hydro’.

In these recommendations, the prefixes ‘hydro’ and ‘dehydro’ are detachable, but are not included in the category of alphabetized detachable prefixes (see P-14.4; see also P-15.1.5.2, P-31.2, P-58.2). This is a change from the recommendations in earlier editions (ref. 1, 2). When along with the endings ‘ene’ and ‘yne’ they are used to modify parent hydrides, they are regulated by the principle of lowest locants, in accord with the numbering of the parent hydride and after priority has been given to indicated hydrogen, added indicated hydrogen, and suffixes, when present, as specified in the general rules for numbering (P-14.4).

P-31.1 THE ENDINGS ‘ENE’ OR ‘YNE’ ENDINGS

P-31.1.1 General methodology

P-31.1.1.1 The presence of one or more double or triple bonds in an otherwise saturated parent hydride [except for parents with Hantzsch-Widman names (see P-22.2.2.1.1), or retained names denoting partial hydrogenation as indicated later (see P-31.2.3.3.1)] is denoted by changing the ending ‘ane’ of the name of a saturated parent hydride to ‘ene’ or ‘yne’. Locants as low as possible are given to multiple bonds as a set, even though this may at times give ‘yne’ endings lower locants than ‘ene’ endings. If a choice remains, preference for low locants is given to the double bonds. In names, the ending ‘ene’ always precedes ‘yne’, with elision of the final letter ‘e’ in ‘ene’. Only the lower locant for a multiple bond is cited, except when the numerical difference between the two locants is greater than one, in which case the higher locant is enclosed in parentheses.

Exceptionally, the endings ‘ene‘ and ‘yne‘ can be added to the ending ‘ane’ in spiro compounds (see SP-2.4, ref. 8), phane nomenclature (see PhII-5.3.1, ref. 6), and ring assemblies (see P-31.1.7 in this book).

If the stereochemistry of a double bond is indicated in a structure it should be specified by *E* or *Z* with the appropriate locant. This includes double bonds in rings of eight or more members (see P-91.2.2).

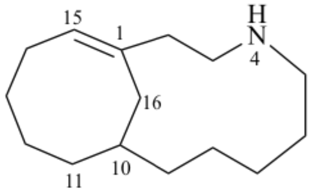
Examples:

$$\overset{1}{C}H_2{=}\overset{2}{C}H\text{-}\overset{3}{C}H_2\text{-}\overset{4}{C}H_3$$
but-1-ene (PIN)

$$H\overset{1}{C}{\equiv}\overset{2}{C}\text{-}\overset{3}{C}H_3$$
propyne (PIN)

$$H\overset{1}{C}{\equiv}\overset{2}{C}\text{-}\overset{3}{C}H{=}\overset{4}{C}H\text{-}\overset{5}{C}H_3$$
pent-3-en-1-yne (PIN)

$$\overset{1}{C}H_2{=}\overset{2}{C}H\text{-}\overset{3}{C}H_2\text{-}\overset{4}{C}{\equiv}\overset{5}{C}H$$
pent-1-en-4-yne (PIN)



4-azabicyclo[8.5.1]hexadec-1(15)-ene (PIN)

P-31.1.1.2 The multiplying prefixes ‘di’, ‘tri’, etc., are placed before endings denoting unsaturation to indicate the number of multiple bonds of each kind, as required, for example, ‘diene’ and ‘triyne’. For euphonic reasons, when the endings ‘ene’ and ‘yne’ are preceded by a multiplying prefix and a locant the letter ‘a’ is inserted. There is no elision of the final letter ‘a’ of a multiplying prefix before ‘ene’ or ‘yne’, for example, ‘tetraene’ and ‘pentayne’.

Examples:

$$\overset{1}{C}H_2{=}\overset{2}{C}H\text{-}\overset{3}{C}H{=}\overset{4}{C}H_2$$
buta-1,3-diene (PIN)

$$\overset{1}{C}H_2{=}\overset{2}{C}H\text{-}\overset{3}{C}H{=}\overset{4}{C}H\text{-}\overset{5}{C}H{=}\overset{6}{C}H\text{-}\overset{7}{C}H{=}\overset{8}{C}H\text{-}\overset{9}{C}H_3$$
nona-1,3,5,7-tetraene (PIN)

P-31.1.1.3 The method of P-31.1.1 is applicable to the following saturated hydrocarbon parent hydrides and to the corresponding hydrides modified by skeletal replacement (‘a’) nomenclature that are described in Chapter P-2:

P-31.1.2 Acyclic parent hydrides
P-31.1.3 Monocyclic parent hydrides
P-31.1.4 Bi- and polycyclic von Baeyer parent hydrides
P-31.1.5 Spiro compounds

P-31.1.6 Phane parent hydrides
P-31.1.7 Ring assemblies of unsaturated components

This method is not used to modify Hantzsch-Widman names for saturated heterocyclic compounds or for totally or partially hydrogenated mancude compounds having retained names, i.e., imidazolidine, morpholine, piperazine, piperidine, pyrazolidine, pyrrolidine (see Table 2.3), quinuclidine (see Table 2.6), and also indane, chromane, isochromane, their chalcogen analogues, and indoline, isoindoline (see Table 3.1). When necessary, the corresponding mancude compounds are modified by using prefixes ‘hydro’ or ‘dehydro’, as indicated in P-31.2, below.

P-31.1.2 Acyclic parent hydrides

P-31.1.2.1 Retained names

The name acetylene is retained for the compound $\mathrm{HC{\equiv}CH}$. It is the preferred IUPAC name, but substitution of any kind is not allowed; however, in general nomenclature, substitution is allowed, for example fluoroacetylene [fluoroethyne (PIN)], but not by alkyl groups or any other group that extends the carbon chain, nor by characteristic groups expressed by suffixes.

The name allene, for $\mathrm{CH_2{=}C{=}CH_2}$, is retained for general nomenclature only; substitution is allowed, but not by alkyl or any other group that extends the carbon chain, nor characteristic groups expressed by suffixes. The systematic name, propa-1,2-diene, is the preferred IUPAC name.

The name isoprene, for $\mathrm{CH_2{=}C(CH_3)\text{-}CH{=}CH_2}$, is retained but only for general nomenclature; no substitution of any kind is allowed. The systematic name, 2-methylbuta-1,3-diene, is the preferred IUPAC name.

The name formazan, for $\overset{1}{\mathrm{HN}}{=}\overset{2}{\mathrm{N}}\text{-}\overset{3}{\mathrm{CH}}{=}\overset{4}{\mathrm{N}}\text{-}\overset{5}{\mathrm{NH_2}}$, is retained and is a preferred IUPAC name fully substitutable by suffixes and prefixes.

The name carbodiimide, for $\mathrm{HN{=}C{=}NH}$, is retained but only for general nomenclature; no substitution of any kind is allowed. The systematic name, methanediimine, is the preferred IUPAC name.

P-31.1.2.2 Systematic names

P-31.1.2.2.1 Homogeneous acyclic parent hydrides and acyclic parent hydrides composed of alternating heteroatoms are modified by the general method of P-31.1.1.

Examples:

$$\overset{1}{\mathrm{CH_3}}\text{-}\overset{2}{\mathrm{CH}}{=}\overset{3}{\mathrm{CH}}\text{-}\overset{4}{\mathrm{CH_2}}\text{-}\overset{5}{\mathrm{CH_2}}\text{-}\overset{6}{\mathrm{CH_3}}$$

hex-2-ene (PIN)

$$\overset{1}{\mathrm{CH_3}}\text{-}\overset{2}{\mathrm{C}}{\equiv}\overset{3}{\mathrm{C}}\text{-}\overset{4}{\mathrm{CH_3}}$$

but-2-yne (PIN)
(not dimethylacetylene)

$$\overset{1}{\mathrm{CH_3}}\text{-}\overset{2}{\mathrm{CH}}{=}\overset{3}{\mathrm{C}}{=}\overset{4}{\mathrm{CH}}\text{-}\overset{5}{\mathrm{CH_2}}\text{-}\overset{6}{\mathrm{CH_3}}$$

hexa-2,3-diene (PIN)
(not 1-ethyl-3-methylallene)

$$\overset{1}{\mathrm{CH_2}}{=}\overset{2}{\mathrm{CH}}\text{-}\overset{3}{\mathrm{CH}}{=}\overset{4}{\mathrm{CH}}\text{-}\overset{5}{\mathrm{C}}{\equiv}\overset{6}{\mathrm{CH}}$$

hexa-1,3-dien-5-yne (PIN)

$$\mathrm{H_2}\overset{1}{\mathrm{N}}\text{-}\overset{2}{\mathrm{N}}{=}\overset{3}{\mathrm{N}}\text{-}\overset{4}{\mathrm{NH}}\text{-}\overset{5}{\mathrm{NH_2}}$$

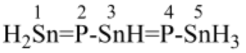
pentaaz-2-ene
(preselected name, see P-12.2)

$$\overset{1}{\mathrm{SiH_3}}\text{-}\overset{2}{\mathrm{SiH}}{=}\overset{3}{\mathrm{SiH}}\text{-}\overset{4}{\mathrm{SiH_2}}\text{-}\overset{5}{\mathrm{SiH_2}}\text{-}\overset{6}{\mathrm{SiH_3}}$$

hexasil-2-ene
(preselected name, see P-12.2)

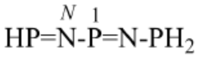
$$\mathrm{H}\overset{1}{\mathrm{Si}}{\equiv}\overset{2}{\mathrm{Si}}\mathrm{H}$$

disilyne
(preselected name, see P-12.2)



$\overset{1}{H_2Sn}=\overset{2}{P}-\overset{3}{SnH}=\overset{4}{P}-\overset{5}{SnH_3}$

tristannaphospha-1,3-diene
(preselected name, see P-12.2)



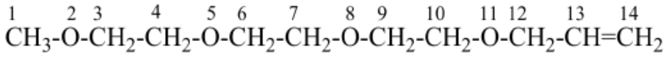
$HP=\overset{N}{N}-\overset{1}{P}=N-PH_2$

N-phosphanylidene-1-(phosphanylimino)phosphanamine
(preselected name, see P-12.2)

P-31.1.2.2.2 Acyclic parent hydrides modified by skeletal replacement (‘a’) nomenclature

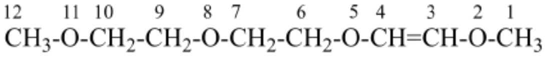
Locants are assigned to unsaturation sites in chains in accordance with the fixed numbering of the hetero chain. If a choice remains, then lowest locants are assigned to unsaturated sites.

Examples:



$\overset{1}{CH_3}-\overset{2}{O}-\overset{3}{CH_2}-\overset{4}{CH_2}-\overset{5}{O}-\overset{6}{CH_2}-\overset{7}{CH_2}-\overset{8}{O}-\overset{9}{CH_2}-\overset{10}{CH_2}-\overset{11}{O}-\overset{12}{CH_2}-\overset{13}{CH}=\overset{14}{CH_2}$

2,5,8,11-tetraoxatetradec-13-ene (PIN)



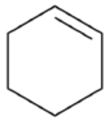
$\overset{12}{CH_3}-\overset{11}{O}-\overset{10}{CH_2}-\overset{9}{CH_2}-\overset{8}{O}-\overset{7}{CH_2}-\overset{6}{CH_2}-\overset{5}{O}-\overset{4}{CH}=\overset{3}{CH}-\overset{2}{O}-\overset{1}{CH_3}$

2,5,8,11-tetraoxadodec-3-ene (PIN)

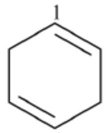
P-31.1.3 Monocyclic parent hydrides

P-31.1.3.1 In monocyclic homogeneous unsaturated compounds, one double or triple bond is always allocated the locant ‘1’. When alone, the locant ‘1’ is omitted in names.

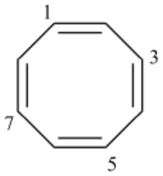
Examples:



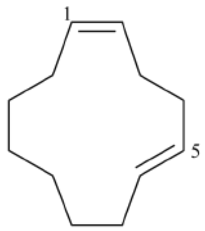
cyclohexene (PIN)



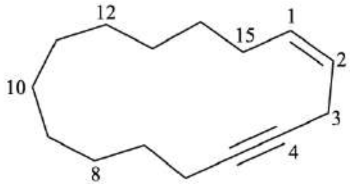
cyclohexa-1,4-diene (PIN)



cycloocta-1,3,5,7-tetraene (PIN)



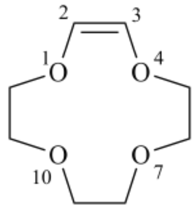
(1Z,5*E*)-cyclododeca-1,5-diene (PIN)



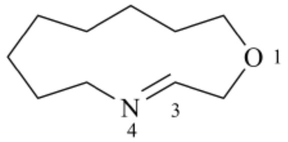
(1*Z*)-cyclopentadec-1-en-4-yne (PIN)

P-31.1.3.2 In rings modified by skeletal replacement (‘a’) nomenclature, low locants are assigned first to heteroatoms and then to unsaturated sites.

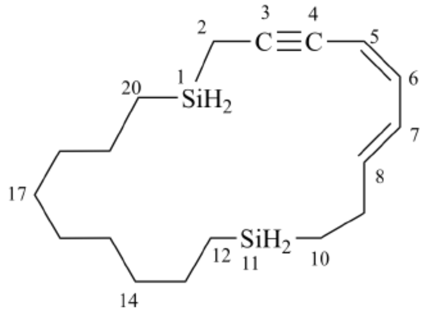
Examples:


2
3
1
O
O
4
O
O
10
7

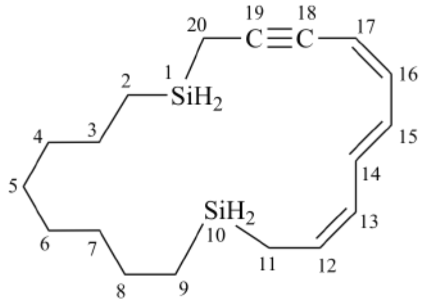
(2*Z*)-1,4,7,10-tetraoxacyclododec-2-ene (PIN)



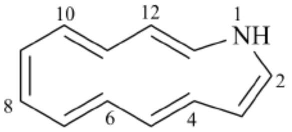
(3*E*)-1-oxa-4-azacyclododec-3-ene (PIN)


3
4
2
C≡C
5
1
6
20
SiH2
7
8
17
SiH2
12
11
10
14

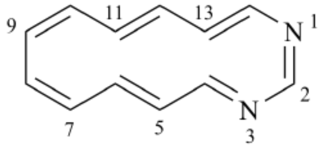
(5*Z*,7*E*)-1,11-disilacycloicosa-5,7-dien-3-yne (PIN)
(not 1,11-disilacycloicosa-4,6-dien-8-yne; the locant set ‘3,5,7’ is lower than ‘4,6,8’)


19
18
20
C≡C
17
1
16
2
SiH2
4
3
15
5
14
SiH2
13
10
6
7
11
12
8
9

(12*Z*,14*E*,16*Z*)-1,10-disilacycloicosa-12,14,16-trien-18-yne (PIN)


10
12
1
NH
2
8
6
4

1-azacyclotrideca-2,4,6,8,10,12-hexaene (PIN)
1*H*-1-aza[13]annulene

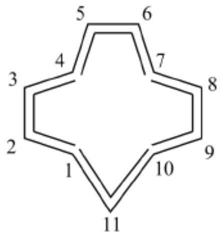

11
13
9
N 1
2
N
3
7
5

1,3-diazacyclotetradeca-1,3,5,7,9,11,13-heptaene (PIN)
1,3-diaza[14]annulene

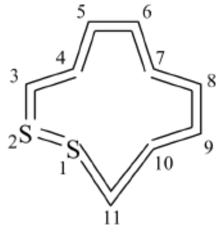
P-31.1.3.3 Cyclic cumulenes

Cyclic cumulenes are composed entirely of atoms, identical or different, linked by double bonds. For homocyclic cumulenes omission of all locants is recommended for preferred IUPAC names (see P-14.3.4.5).

Examples:



cycloundecaundecaene (PIN)

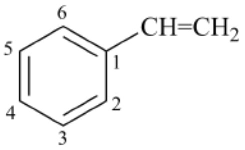


$1\lambda^4$,$2\lambda^4$-dithiacycloundecaundecaene (PIN)

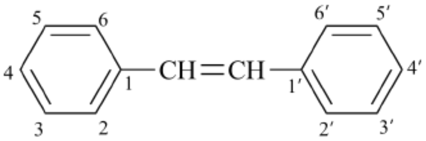
P-31.1.3.4 Retained names.

Styrene, stilbene, and fulvene are the only retained names for parent hydrides containing a monocyclic ring system and side-chain unsaturation. All are used only in general nomenclature. Styrene and stilbene can be substituted only on the ring and only as prescribed in P-15.1.8.2.2; fulvene cannot be substituted at all.

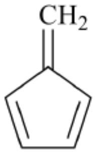
Examples:



styrene (ring substitution only)
ethenylbenzene (PIN)



stilbene (ring substitution only)
1,1′-(ethene-1,2-diyl)dibenzene (PIN)



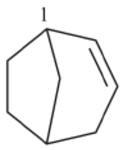
fulvene (no substitution)
5-methylidenecyclopenta-1,3-diene (PIN)

P-31.1.4 Bi- and polycyclic von Baeyer parent hydrides

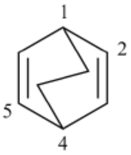
It should be noted that some bi- and polycyclic von Baeyer parent hydrides qualify for phane names as preferred IUPAC names (see P-52.2.5).

P-31.1.4.1 Low locants are allocated first in accordance with the fixed numbering of the ring system. Low locants are allocated for double bonds when the atoms of each bond have consecutive locants.

Examples:



bicyclo[3.2.1]oct-2-ene (PIN)



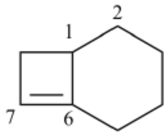
bicyclo[2.2.2]octa-2,5-diene (PIN)

P-31.1.4.2 If there is a choice of names and numbering, the following criteria are considered in order until a decision is reached:

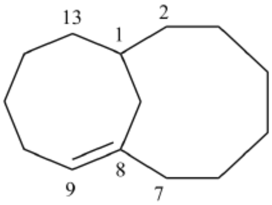
(1) a minimum number of compound locants. A compound locant is used for a double bond if the locants of the atoms at each end of the bond do not differ by a value of one. When a compound locant is required, the higher locant is cited in parentheses. A benzene ring is shown and described as a cyclohexatriene corresponding to the Kekulé structure. Other aromatic rings are treated similarly, when required;

Note: The seniority of single locants over compound locants was established in 1989 for numbering steroids [see S3-2.5 (2), ref. 16] and extended to von Baeyer systems in the 1999 publication on von Baeyer nomenclature (see VB-8.3.1, ref. 7).

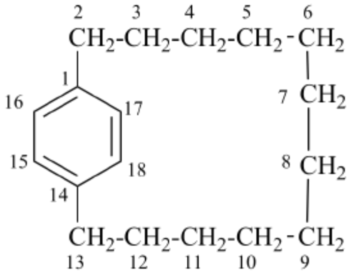
Examples:



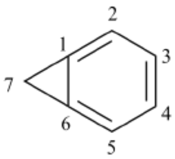
bicyclo[4.2.0]oct-6-ene (PIN)
[not bicyclo[4.2.0]oct-1(8)-ene]



bicyclo[6.5.1]tetradec-8-ene (PIN)
[not bicyclo[6.5.1]tetradec-1(13)-ene]



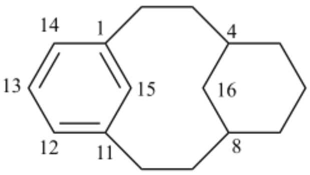
bicyclo[12.2.2]octadeca-1(16),14,17-triene
[not bicyclo[12.2.2]octadeca-1(17),14(18),15-triene]
1(1,4)-benzenacyclotridecaphane (PIN, see P-52.2.5)



bicyclo[4.1.0]hepta-1,3,5-triene (PIN)
[not bicyclo[4.1.0]hepta-1(6),2,4-triene]

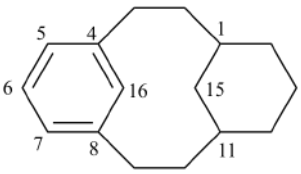
(2) when comparing double bond locants that also include compound locants, any number in parentheses is ignored;

Examples:

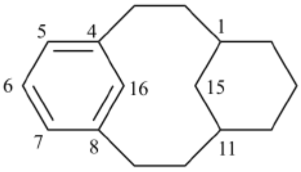


(I)

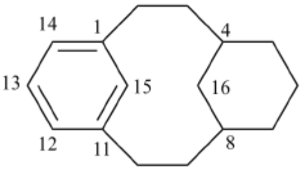
not



(II)

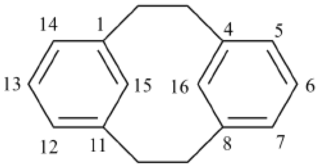
nor 

(**III**)

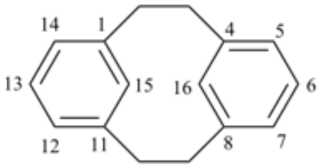
nor 

(**IV**)

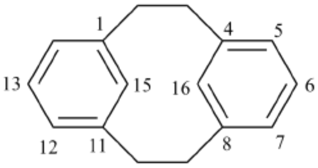
tricyclo[9.3.1.$1^{4,8}$]hexadeca-1(15),11,13-triene (**I**)
[not tricyclo[9.3.1.$1^{4,8}$]hexadeca-4(16),5,7-triene (**II**);
nor tricyclo[9.3.1.$1^{4,8}$]hexadeca-4,6,8(16)-triene (**III**);
nor tricyclo[9.3.1.$1^{4,8}$]hexadeca-1(14),11(15),12-triene (**IV**);
the set of locants ‘1,11,13’ in (**I**) is lower than ‘4,5,7’ in (**II**) or ‘4,6,8’ in (**III**);
and (**IV**) has two compound locants whereas (**I**) has only one compound locant]
1(1,3)-benzena-4(1,3)-cyclohexanacyclohexaphane (PIN, see P-52.2.5)



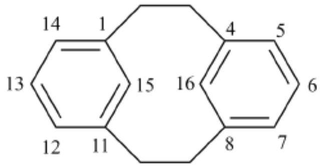
(**I**)

not 

(**II**)

nor 

(**III**)

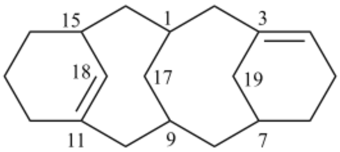
nor 

(**IV**)

tricyclo[9.3.1.$1^{4,8}$]hexadeca-1(15),4(16),5,7,11,13-hexaene (**I**)
not tricyclo[9.3.1.$1^{4,8}$]hexadeca-1(15),4,6,8(16),11,13-hexaene (**II**);
nor tricyclo[9.3.1.$1^{4,8}$]hexadeca-1(14),4,6,8(16),11(15),12-hexaene (**III**);
nor tricyclo[9.3.1.14,8]hexadeca-1(14),4(16),5,7,11(15),12-hexaene (**IV**)
the set of locants in (**I**) ‘1,4,5,7,11,13’ is lower than ‘1,4,6,8,11,13’ in **II**);
also name (**I**) has two compound locants compared to three in names (**III**) and **IV**)]
1,4(1,3)-dibenzenacyclohexaphane (PIN, see P-52.2.5)

(3) if there is still a choice, low locants are selected considering all locants (including those in parentheses) as a set.

Example:

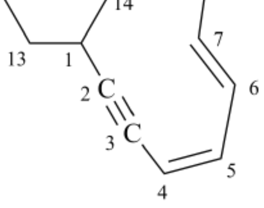


tetracyclo[7.7.1.$1^{3,7}$.$1^{11,15}$]nonadeca-3,11(18)-diene (PIN)
[not tetracyclo[7.7.1.$1^{3,7}$.$1^{11,15}$]nonadeca-3(19),11-diene;
the locant set ‘3,11,18’ is lower than ‘3,11,19’]

P-31.1.4.3 Bi- and polycyclic von Baeyer structures with both double and triple bonds. If both double and triple bonds are present, the following criteria for numbering are considered, in order, until a decision is reached:

(1) compound locants are kept to a minimum.

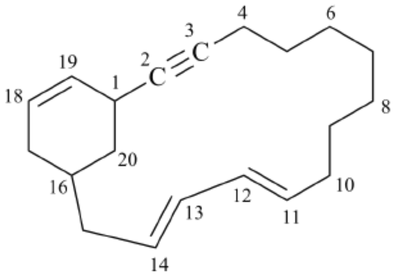
Example:



(4*Z*,6*E*)-bicyclo[8.3.1]tetradeca-4,6,10-trien-2-yne (PIN)
(not bicyclo[8.3.1]tetradeca-1(13),4,6-trien-8-yne)

(2) lower locants are assigned to multiple bonds as a set;

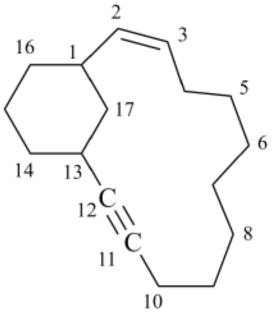
Example:



(11*E*,13*E*)-bicyclo[14.3.1]icosa-11,13,18-trien-2-yne (PIN)
(not bicyclo[14.3.1]icosa-3,5,17-trien-14-yne;
the locant set '2,11,13,18' is lower than '3,5,14,17')

(3) lower locants are assigned to double bonds;

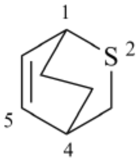
Example:



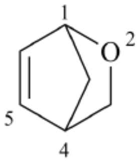
(2*Z*)-bicyclo[11.3.1]heptadec-2-en-11-yne (PIN)
(not bicyclo[11.3.1]heptadec-11-en-2-yne)

P-31.1.4.4 Bi- and polycyclic von Baeyer heterocycles named by skeletal replacement ('a') nomenclature. In heterocyclic compounds formed using skeletal replacement ('a') nomenclature, low locants are assigned to heteroatoms, in accord with the fixed numbering of the system, then to unsaturated sites.

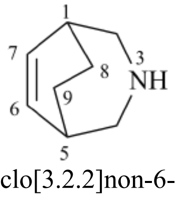
Examples:



2-thiabicyclo[2.2.2]oct-5-ene (PIN)



2-oxabicyclo[2.2.1]hept-5-ene (PIN)



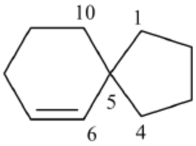
3-azabicyclo[3.2.2]non-6-ene (PIN)

P-31.1.5 Spiro compounds

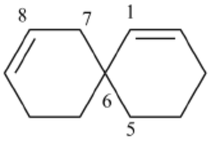
P-31.1.5.1 Spiro compounds composed of unsaturated rings

P-31.1.5.1.1 Low locants are assigned to double bonds in accordance with the fixed numbering of the spiro compound.

Examples:



spiro[4.5]dec-6-ene (PIN)

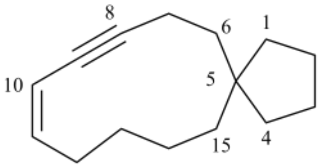


spiro[5.5]undeca-1,8-diene (PIN)

P-31.1.5.1.2 If there are double and triple bonds present, the following criteria are considered, in order, until a decision is reached:

(1) lower locants are assigned to multiple bonds as a set;

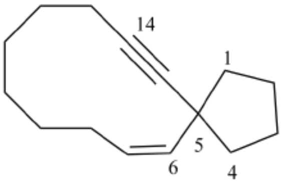
Example:



(10*Z*)-spiro[4.10]pentadec-10-en-8-yne (PIN)

(2) if there is still a choice, low locants are assigned to double bonds.

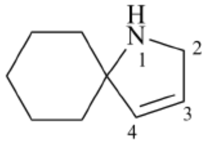
Example:



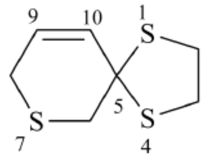
(6*Z*)-spiro[4.10]pentadec-6-en-14-yne (PIN)

P-31.1.5.1.3 Heteroatoms in spiro compounds consisting of monocyclic rings denoted by skeletal replacement (‘a’) nomenclature have priority for low locants.

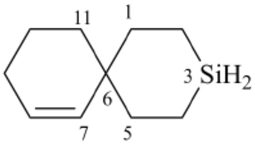
Examples:



1-azaspiro[4.5]dec-3-ene (PIN)



1,4,7-trithiaspiro[4.5]dec-9-ene (PIN)



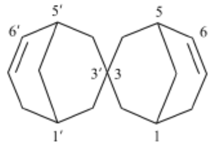
3-silaspiro[5.5]undec-7-ene (PIN)

P-31.1.5.2 Spiro compounds consisting of saturated polycyclic von Baeyer components.

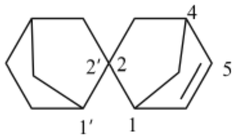
P-31.1.5.2.1 Unsaturation in a saturated spiro ring system with components named by the von Baeyer system is indicated by the endings ‘ene’ and the multiplicative prefixes ‘di’, ‘tri’, etc. when required; the ending ‘ene’ is cited after the last bracket of the spiro name. The final letter ‘e’ of the saturated hydrocarbon name is elided if followed by a vowel. If there is a choice, low locants are assigned, in order, to spiro junction(s), heteroatoms and double bonds (see SP-2.4 in ref. 8).

Note: The placement location of the ‘ene’ endings after the closing brackets around the parent spiro name was established in the publication on nomenclature of spiro compounds (ref. 8)

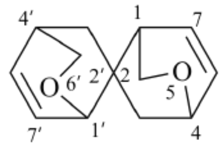
Examples:



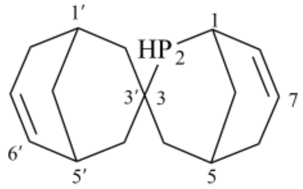
3,3′-spirobi[bicyclo[3.3.1]nonane]-6,6′-diene (PIN)



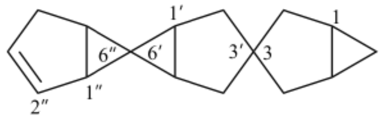
2,2′-spirobi[bicyclo[2.2.1]heptan]-5-ene (PIN)



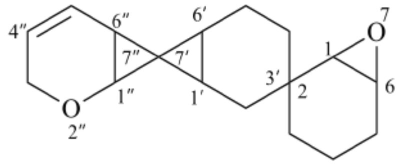
5,6′-dioxa-2,2′-spirobi[bicyclo[2.2.2]octane]-7,7′-diene (PIN)



2-phospha-3,3′-spirobi[bicyclo[3.3.1]nonane]-6′,7-diene (PIN)



3,3′:6′,6″-dispiroter[bicyclo[3.1.0]hexan]-2″-ene (PIN)



2″,7-dioxa-2,3′:7′,7″-dispiroter[bicyclo[4.1.0]heptan]-4″-ene (PIN)
[not 5″,7-dioxa-2,3′:7′,7″-dispiroter[bicyclo[4.1.0]heptan]-2″-ene;
the locant set ‘2″,7’ is lower than ‘5″,7’ for the ‘oxa’ prefixes]

P-31.1.6 Phane parent hydrides

P-31.1.6.1 Double bonds in amplificants and in simplified phane skeletons

The presence of one or more double or triple bonds in an otherwise saturated phane parent hydride, except in amplificants with Hantzsch-Widman names, is denoted by changing the final letter ‘e’ of the phane parent hydride name to ‘ene’ or ‘yne’, with appropriate multiplying prefixes to indicate the multiplicity of each kind of unsaturated site (ref. 6, PhII-5.3).

Low locants are allocated for double or triple bonds in accordance with the fixed numbering of the phane parent hydride and of phane parent hydrides modified by skeletal replacement (‘a’) nomenclature. Three types of locants are used to fully describe compounds derived from phane parent hydrides:

(1) primary locants, i.e. arabic number locants that denote the atoms and superatoms of the phane parent skeleton;

(2) composite locants, i.e. primary locants with a superscript arabic number locant denoting positions in amplificants (see P-26.4.3);

(3) compound locants, which are primary or composite locants followed by another locant in parentheses, indicating that a double bond is not located between two consecutive locants.

In phane nomenclature, double and triple bonds are denoted in two ways:

(1) by the lowest locant of a double or triple bond when two consecutive locants are:

(a) primary locants; or

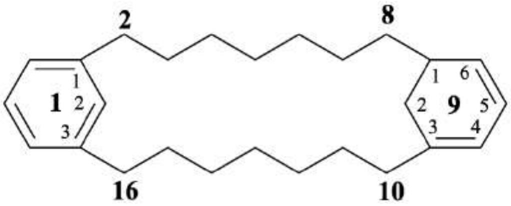
(b) composite locants;

(2) by a compound locant, when two locants are not consecutive, or when one is a primary locant and the other is a composite locant..

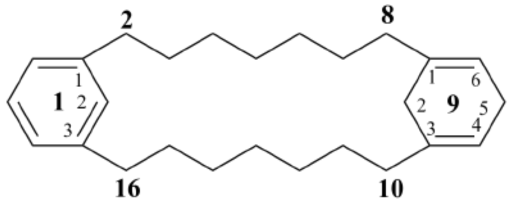
If there is a choice the criteria of P-31.1.4.3 are applied.

This is a change from PhII-5.3.2.

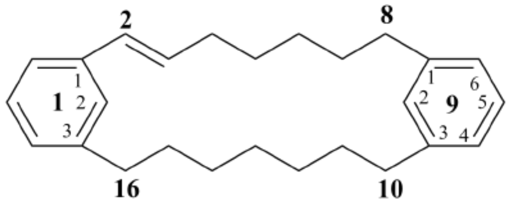
Examples:



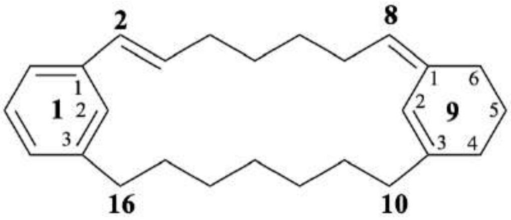
1(1,3)-benzena-9(1,3)-cyclohexanacyclohexadecaphane-9^3,9^5-diene (PIN)
not 1(1,3)-benzena-9(1,3)-cyclohexanacyclohexadecaphane-9^1(9^6),9^4-diene



1(1,3)-benzena-9(1,3)-cyclohexanacyclohexadecaphane-9^1(9^6),9^3-diene (PIN)



1,9(1,3)-dibenzenacyclohexadecaphan-2-ene (PIN)

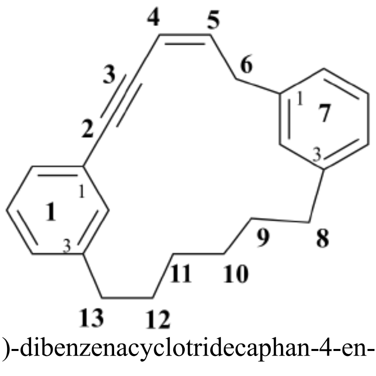


(2*E*,8(9^1)*Z*)-1(1,3)-benzena-9(1,3)-cyclohexanacyclhexadecaphan-2,8(9^1),9^2-triene

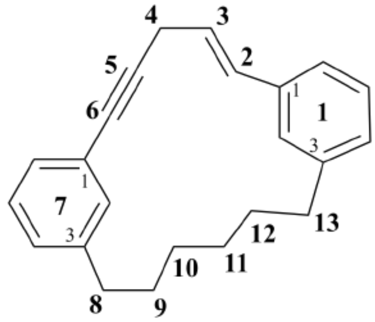
P-31.1.6.2 Phane structures with both double and triple bonds

Double and triple bonds in a phane structure are described by the method of P-31.1.4.3. Low locants are allocated to double and triple bonds first when considered together as a set in ascending order and, if a choice is still needed, to double bonds.

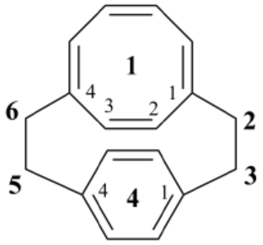
Examples:



(4*Z*)-1,7(1,3)-dibenzenacyclotridecaphan-4-en-2-yne (PIN)



(2*E*)-1,7(1,3)-dibenzenacyclotridecaphan-2-en-5-yne (PIN)



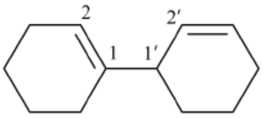
1(1,4)-cyclooctana-4(1,4)-benzenacyclohexaphane-1^1(1^8),1^2,1^4,1^6-tetraene (PIN)

P-31.1.7 Ring assemblies of unsaturated components.

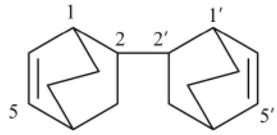
P-31.1.7.1 Unsaturation in ring assemblies composed of saturated components, monocyclic or alicyclic, is indicated by the endings ‘ene’, ‘yne’, etc. and the multiplicative prefixes ‘di’, ‘tri’, etc; the endings are cited after the last bracket of the ring assembly name. The final letter ‘e’ of the saturated hydrocarbon name is elided if followed by a vowel. If there is a choice, low locants are assigned, in order, to ring assembly junction(s), heteroatoms and multiple bonds (see also P-31.1.5.2).

The location of the ‘ene’, ‘yne’, etc., endings after the closing brackets of the ring assembly name is a change from the 1979 and the 1993 Guide editions (ref. 1, 2) and is completely consistent with the method established for spiro compounds in the 1999 publication on nomenclature of spiro compounds (ref. 8)

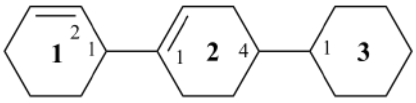
Examples:



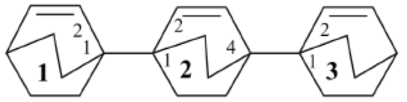
[1,1′-bi(cyclohexane)]-1,2′-diene (PIN)



[2,2′-bi(bicyclo[2.2.2]octane)]-5,5′-diene (PIN)



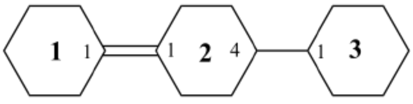
[1^1,2^1:2^4,3^1-tercyclohexane]-1^2,2^1-diene (PIN)
[1,1′:4′,1″-tercyclohexane]-1′,2-diene



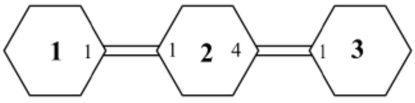
[1^1,2^1:2^4,3^1-terbicyclo[2.2.2]octane]-1^2,2^2,3^2-triene (PIN)
[1,1′:4′,1″-terbicyclo[2.2.2]octane]-2,2′,2″-triene

P-31.1.7.2 Double bonds linking two rings or ring systems are named in the same way as ring assemblies composed of three or more saturated components. Locants for the terminal position of such bonds are enclosed in parentheses (compound locants).

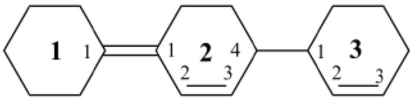
Examples:



[^{1},2^1:2^4,3^1-tercyclohexan]-1^1(2^1)-ene (PIN)
[1,1′:4′,1″-tercyclohexan]-1(1′)-ene



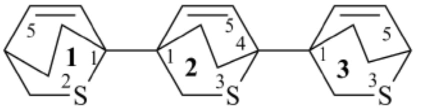
[1^1,2^1:2^4,3^1-tercyclohexane]-1^1(2^1),2^4(3^1)-diene (P IN)
[1,1′:4′,1″-tercyclohexane]-1(1′),4′(1″)-diene



[1^1,2^1:2^4,3^1-tercyclohexane]-1^1(2^1),2^2,3^2- triene (PIN)
[1,1′:4′,1″-tercyclohexane]-1(1′),2′,2″-triene

P-31.1.7.3 When heterocyclic ring assemblies consisting of monocyclic, bi- or polyalicyclic components are named by skeletal replacement (‘a’) nomenclature, low locants are assigned, in order, to ring junctions, heteroatoms and then unsaturation sites.

Example:



1^2,2^3,3^3-trithia[1^1,2^1:2^4,3^1-terbicyclo[2.2.2]octane]-1^5,2^5,3^5-triene (PIN)
2,3′,3″-trithia-[1,1′:4′,1″-terbicyclo[2.2.2]octane]-5,5′,5″-triene

P-31.2 SUBSTITUENT GROUPS MODIFIED BY THE PREFIXES ‘HYDRO’ OR ‘DEHYDRO’

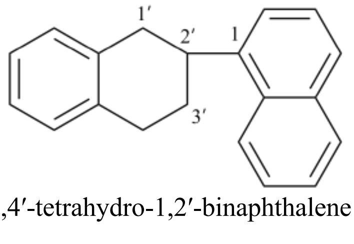
P-31.2.1 The prefixes ‘hydro/dehydro’ are used to indicate addition and subtraction, respectively, of hydrogen atoms to or from mancude compounds. ‘Hydro’ and ‘dehydro’ prefixes are detachable prefixes but are not included in those prefixes that are cited in alphanumerical order. Thus, in names, they are cited immediately at the front of the name of the parent hydride, after alphabetized prefixes and before nondetachable prefixes.

> This is a change from previous recommendations. In these recommendations the prefixes ‘hydro’ and ‘dehydro’ are detachable but not alphabetized with other substituent prefixes. In names, they are cited immediately before the name of the parent hydride, after alphabetized prefixes and before nondetachable prefixes.

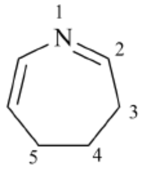
The starting point and direction of numbering of a compound are chosen so as to give lowest locants to fixed numbering of a polycyclic ring system, as in naphthalene, quinoline, etc., then to heteroatoms in heterocycles, and then to indicated hydrogen, when present, in accordance with the methodology described in P-14.4 for the construction of substitutive names.

P-31.2.2 General methodology

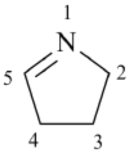
‘Hydro’ and ‘dehydro’ prefixes are associated with hydrogenation and dehydrogenation, respectively, of a double bond; thus, multiplying prefixes of even values, as ‘di’, ‘tetra’, etc. are used to indicate the saturation of double bond(s), for example ‘dihydro’, ‘tetrahydro’; or creation of double (or triple) bonds, as ‘didehydro’, etc.. In names, they are placed immediately at the front of the name of the parent hydride and in front of any nondetachable prefixes. Indicated hydrogen atoms have priority over ‘hydro‘ prefixes for low locants. If indicated hydrogen atoms are present in a name, the ‘hydro‘ prefixes precede them.



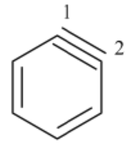
1′,2′,3′,4′-tetrahydro-1,2′-binaphthalene (PIN)



4,5-dihydro-3*H*-azepine (PIN)



3,4-dihydro-2*H*-pyrrole (PIN)

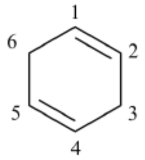


1,2-didehydrobenzene (PIN, see P-31.2.4.1)
cyclohex-1,3-dien-5-yne
(not benzyne)

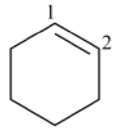
P-31.2.3 The prefix ‘hydro’

P-31.2.3.1 ‘Hydro’ prefixes are used to modify the degree of hydrogenation of monocyclic mancude compounds having retained or systematic names, except for the hydro derivatives of benzene, for which the traditional names ‘cyclohexene’ and ‘cyclohexadiene’ are the preferred IUPAC names.

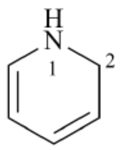
Examples:



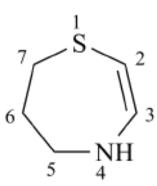
cyclohexa-1,4-diene (PIN)
(not 1,4-dihydrobenzene)



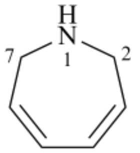
cyclohexene (PIN)
(not 1,2,3,4-tetrahydrobenzene)



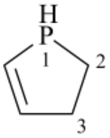
1,2-dihydropyridine (PIN)



4,5,6,7-tetrahydro-1,4-thiazepine (PIN)



2,7-dihydro-1*H*-azepine (PIN)

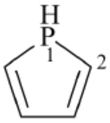


2,3-dihydro-1*H*-phosphole (PIN)

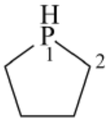
P-31.2.3.2 Names of saturated heteromonocyclic compounds

Preferred IUPAC names of saturated heteromonocyclic compounds are either Hantzsch-Widman names described in P-22.2.2.1.1 or retained names described in Table 2.3. Names of saturated rings derived by using hydro prefixes from Hantzsch-Widman names, retained names modified by adding the maximum of hydro prefixes, or 'cyclo' names described in P-22.2.5 are not preferred IUPAC names, but they may be used in general nomenclature.

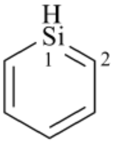
Examples:



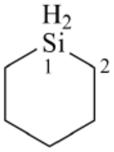
1*H*-phosphole (PIN)



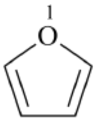
phospholane (PIN)
tetrahydro-1*H*-phosphole



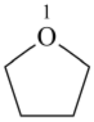
siline (PIN)



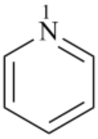
silinane (PIN)
hexahydrosiline



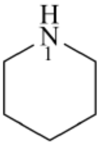
furan (PIN)



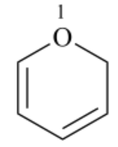
oxolane (PIN)
tetrahydrofuran



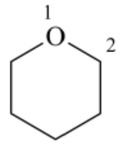
pyridine (PIN)



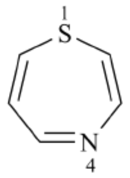
piperidine (PIN)
hexahydropyridine



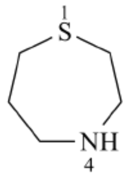
2*H*-pyran (PIN)



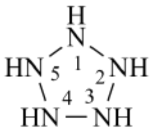
oxane (PIN)
tetrahydropyran



1,4-thiazepine (PIN)



1,4-thiazepane (PIN)
hexahydro-1,4-thiazepine



cyclopentaazane
pentazolidine (preselected name;
see P-12.1; P-22.2.2.1.5.2; P-22.2.5)

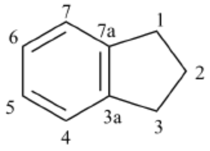
P-31.2.3.3 Saturation of double bonds in polycyclic mancude compounds

P-31.2.3.3.1 Retained names of partially saturated polycyclic mancude compounds
P-31.2.3.3.2 Polycyclic mancude compounds
P-31.2.3.3.3 Spiro compounds
P-31.2.3.3.4 Phane compounds
P-31.2.3.3.5 Ring assemblies

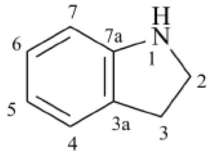
P-31.2.3.3.1 Retained names of partially saturated polycyclic mancude compounds

Names listed in Table 3.1 are retained names that are not used as preferred IUPAC names. They are, however acceptable in general nomenclature with full substitution, including characteristic groups expressed as suffixes, but not as fusion components nor as amplificants in Phane Nomenclature.

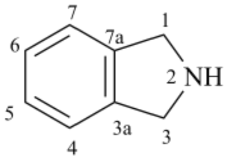
Table 3.1 Retained names of partially saturated polycyclic parent hydrides



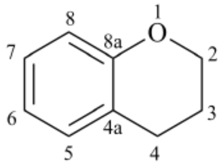
indane
(formerly indan)
2,3-dihydro-1*H*-indene (PIN)



1*H*-indoline
2,3-dihydro-1*H*-indole (PIN)



2*H*-isoindoline
2,3-dihydro-1*H*-isoindole (PIN)

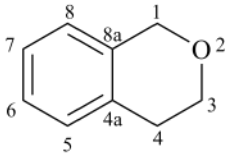


chromane
3,4-dihydro-2*H*-1-benzopyran (PIN)
3,4-dihydro-2*H*-chromene

thiochromane (S instead of O)
3,4-dihydro-2*H*-1-benzothiopyran (PIN)
3,4-dihydro-2*H*-thiochromene

selenochromane (Se instead of O)
3,4-dihydro-2*H*-1-benzoselenopyran (PIN)
3,4-dihydro-2*H*-selenochromene

tellurochromane (Te instead of O)
3,4-dihydro-2*H*-1-benzotelluropyran (PIN)
3,4-dihydro-2*H*-tellurochromene



isochromane
3,4-dihydro-1*H*-2-benzopyran (PIN)
3,4-dihydro-1*H*-isochromene

isothiochromane (S instead of O)
3,4-dihydro-1*H*-2-benzothiopyran (PIN)
3,4-dihydro-1*H*-isothiochromene

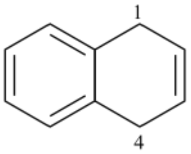
isoselenochromane (Se instead of O)
3,4-dihydro-1*H*-2-benzoselenopyran (PIN)
3,4-dihydro-1*H*-isoselenochromene

isotellurochromane (Te instead of O)
3,4-dihydro-1*H*-2-benzotelluropyran (PIN)
3,4-dihydro-1*H*-isotellurochromene

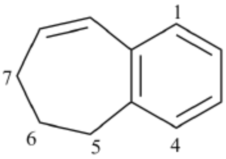
P-31.2.3.3.2 Polycyclic mancude compounds

The degree of hydrogenation of partially or fully saturated individual mancude ring systems, carbocyclic or heterocyclic, is given by 'hydro' prefixes, in accordance with the general methodology described in P-31.2.2. Total hydrogenation is indicated by the appropriate multiplicative prefixes indicating the total number of hydrogen atoms attached, but locants are omitted (see P-14.3.4.5).

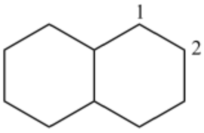
Examples:



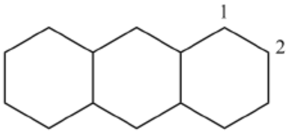
1,4-dihydronaphthalene (PIN)



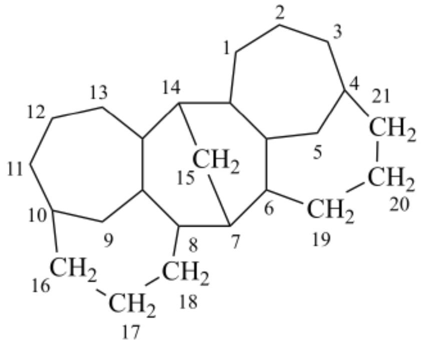
6,7-dihydro-5*H*-benzo[7]annulene (PIN)



decahydronaphthalene (PIN)



tetradecahydroanthracene (PIN)

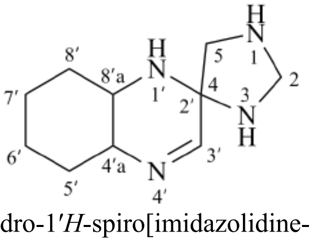

1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17
18
19
20
21
CH2

octadecahydro-7,14-methano-4,6:8,10-dipropanodicyclohepta[*a*,*d*][8]annulene (PIN)
hexacyclo[$15.3.2.2^{3,7}.1^{2,12}.0^{13,21}.0^{11,25}$]pentacosane (see P-23.2.6.3)

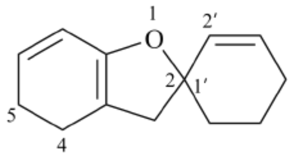
P-31.2.3.3.3 Spiro compounds

Spiro compounds including mancude components are modified in accordance with the general methodology described in P-31.2.2.

Examples:


H
N
1
2
3
N
H
4
5
8′
8′a
H
N
1′
2′
3′
N
4′
4′a
5′
6′
7′

4′a,5′,6′,7′,8′,8′a-hexahydro-1′*H*-spiro[imidazolidine-4,2′-quinoxaline] (PIN)



4,5-dihydro-3*H*-spiro[[1]benzofuran-2,1′-cyclohexan]-2′-ene (PIN)

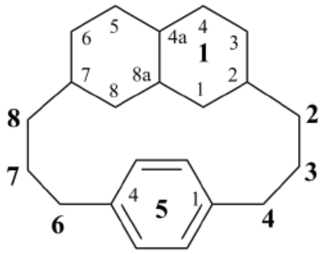
P-31.2.3.3.4 Phane compounds

When the name of an amplificant implies the presence of a maximum number of noncumulated double bonds, other states of hydrogenation are indicated by use of the prefix ‘hydro’. This method is applied as follows (see ref. 6, PhII-5.1 and PhII-5.2):

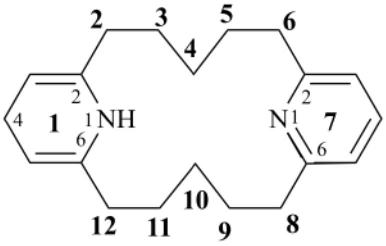
(1) ‘Hydro’ prefixes are used to modify mancude heteromonocycles having retained names or named in accordance with the extended Hantzsch-Widman system. However, names for the fully saturated heteromonocycles that have retained names or Hantzsch-Widman names are preferred to those expressed by ‘hydro’ prefixes, for example, oxolane and piperidine are preferred to tetrahydrofuran and hexahydropyridine, respectively.

(2) ‘Hydro’ prefixes are used to indicate all modifications of the degree of unsaturation of carbocyclic or heterocyclic mancude parent hydrides, except for benzene. Retained names of partially hydrogenated parent hydrides, such as indane and chromane (see P-31.2.3.3.1), are not recommended as amplificants in phane nomenclature.

Examples:



$1^1,1^2,1^3,1^4,1^{4a},1^5,1^6,1^7,1^8,1^{8a}$-decahydro-1(2,7)-naphthalena-5(1,4)-benzenacyclooctaphane (PIN)



$1^1,1^4$-dihydro-1,7(2,6)-dipyridinacyclododecaphane (PIN)

P-31.2.3.3.5 Ring assemblies

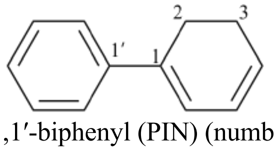
The degree of hydrogenation of ring assemblies composed of mancude components is given by ‘hydro’ prefixes, in accordance with the general methodology described in P-31.2.2. Since assemblies are considered as parent hydrides, the degree of hydrogenation of the different components can be modified, to a certain extent, in a way that is not allowed for the individual components. This is the case of assemblies composed of monocyclic components, in which the names are different for the mancude and the saturated component. Thus, assemblies composed of monocyclic components and those composed of ring system components are treated differently.

P-31.2.3.3.5.1 Ring assemblies composed of monocyclic components
P-31.2.3.3.5.2 Ring assemblies composed of ring systems

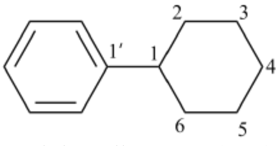
P-31.2.3.3.5.1 Ring assemblies composed of monocyclic components

(a) Ring assemblies composed of monocyclic mancude or saturated hydrocarbons. Low locants are assigned to ‘hydro’ prefixes in accordance with the fixed numbering of each assembly. In biphenyl and polyphenyl assemblies, one benzene ring must remain in the assembly; otherwise, the starting parent hydride is the saturated assembly and the ending ‘ene’ is used to denote unsaturation (see P-31.1.7). Furthermore, when a modified ring assembly of two rings consists of a benzene ring and a cyclohexane ring substitutive nomenclature is preferred (see P-54.3).

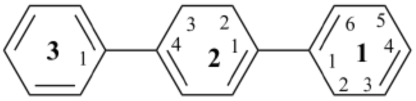
Examples:



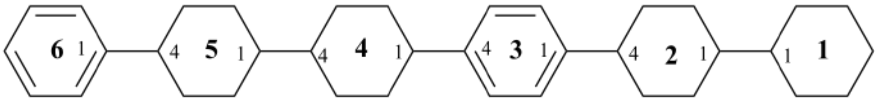
2,3-dihydro-1,1′-biphenyl (PIN) (numbering shown)
(cyclohexa-1,3-dien-1-yl)benzene



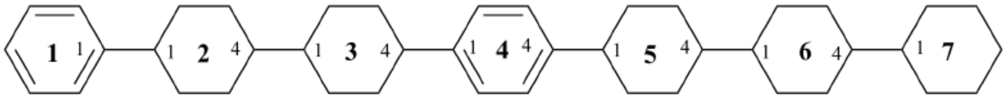
cyclohexylbenzene (PIN)
1,2,3,4,5,6-hexahydro-1,1′-biphenyl (numbering shown)



$1^2,1^5,2^2,2^3$-tetrahydro-$1^1,2^1{:}2^4,3^1$-terphenyl (PIN)
2,2′,3′,5-tetrahydro-1,1′:4′,1″-terphenyl
[4-(cyclohexa-1,4-dien-1-yl)cyclohexa-1,3-dien-1-yl]benzene
(substitutive name)



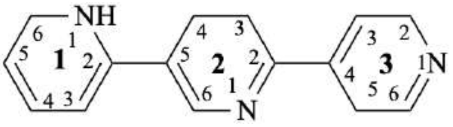
$1^1,1^2,1^3,1^4,1^5,1^6,2^1,2^2,2^3,2^4,2^5,2^6,4^1,4^2,4^3,4^4,4^5,4^6,5^1,5^2,5^3,5^4,5^5,5^6$-tetracosahydro-$1^1,2^1{:}2^4,3^1{:}3^4,4^1{:}4^4,5^1{:}5^4,6^1$-sexiphenyl
(PIN)
1,1′,1‴,1‴ ′,2,2′,2‴,2‴ ′,3,3′,3‴,3‴ ′,4,4′,4‴,4‴ ′,5,5′,5‴,5‴ ′,6,6′,6‴,6‴ ′-tetracosahydro-
1,1′:4′,1″:4″,1‴:4‴ ′1‴ ′:4‴ ′,1‴ ″-sexiphenyl
4-[4-([1,1′-bi(cyclohexan)]-4-yl)phenyl]-4′-phenyl-1,1′-bi(cyclohexane) (substitutive name)
{not 1-($2^1,2^2,2^3,2^4,2^5,2^6,3^1,3^2,3^3,3^4,3^5,3^6$-dodecahydro[$1^1,2^1{:}2^4,3^1$-terphenyl]-$1^4$-yl)-4-([1,1′-bi(cyclohexan)]-4-yl)benzene (substitutive name)}
Note: According to P-52.2.5.1, seven nodes are required for a phane name.



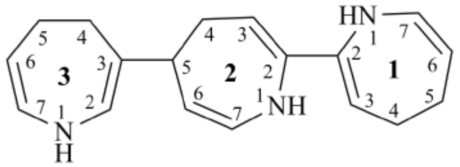
1(1),4(1,4)-dibenzena-2,3,5,6(1,4),7(1)-pentacyclohexanaheptaphane (PIN; numbering shown)
4-[4-(4′-phenyl[1,1′-bi(cyclohexan)]-4-yl)phenyl)-11,21:24,31-tercyclohexane (substitutive name)
4-[4-(4′-phenyl[1,1-bi(cyclohexan)]-4-yl)pheny]-1,1′:4′,1″-tercyclohexane (substitutive name)

(b) Ring assemblies composed of heteromonocycles. Low locants are assigned to junctions between rings, then to indicated hydrogen, if any, and finally to 'hydro' prefixes.

Examples:



$1^1,1^6,2^3,2^4,3^2,3^5$-hexahydro-$1^2,2^5{:}2^2,3^4$-terpyridine (PIN)
1,2″,3′,4′,5″,6-hexahydro-2,5′:2′,4″-terpyridine

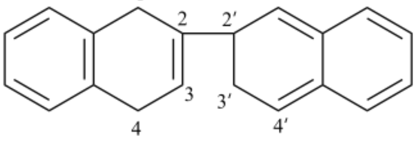


$1^4,1^5,2^4,2^5,3^4,3^5$-hexahydro-$1^1\mathit{H},2^1\mathit{H},3^1\mathit{H}$-$1^2,2^2{:}2^5,3^3$-terazepine (PIN)
4,4′,4″,5,5′,5″-hexahydro-1*H*,1′*H*,1″*H*-2,2′:5′,3″-terazepine

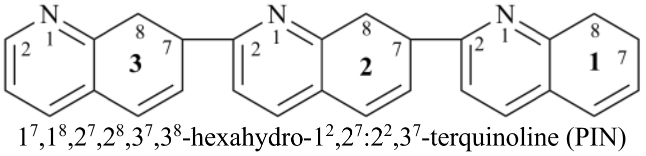
P-31.2.3.3.5.2 Ring assemblies composed of polycyclic compounds

Low locants are assigned to the junctions between components, then to indicated hydrogen atoms, if any, and finally to 'hydro' prefixes.

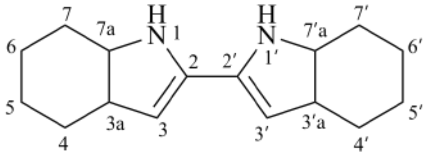
Examples:



1,2′,3′,4-tetrahydro-2,2′-binaphthalene (PIN)



$1^7,1^8,2^7,2^8,3^7,3^8$-hexahydro-$1^2,2^7{:}2^2,3^7$-terquinoline (PIN)
7,7′,7″,8,8′,8″-hexahydro-2,7′:2′,7″-terquinoline

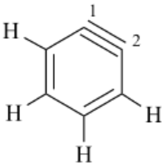


3a,3′a,4,4′,5,5′,6,6′,7,7′,7a,7′a-dodecahydro-1*H*,1′*H*-2,2′-biindole (PIN)

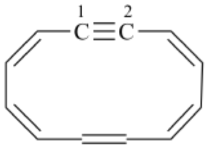
P-31.2.4 The prefix ‘dehydro’

P-31.2.4.1 The subtractive prefix ‘dehydro’ is used to denote the removal of hydrogen atoms and the formation of multiple bonds. Its use is very limited in systematic nomenclature of organic compounds. Applied to benzene, it leads to the name ‘1,2-didehydrobenzene’, the preferred IUPAC name, rather than ‘benzyne’ that was formerly used. Applied to annulenes, it leads to didehydro[*n*]annulenes that are not used in preferred IUPAC names, but are acceptable for use in general nomenclature.

Examples:



1,2-didehydrobenzene (PIN)
cyclohexa-1,3-dien-5-yne
(formerly called ‘benzyne’)

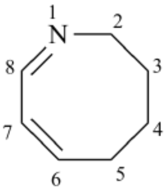


1,2-didehydro[12]annulene (numbering shown)
cyclododeca-1,3,5,7,9-pentaen-11-yne (PIN)

P-31.2.4.2 The ‘dehydro’ prefix is more widely used in natural product nomenclature in order to preserve semisystematic names of stereoparents (see P-101.6). It is also used in the nomenclature of carbohydrates (ref. 27).

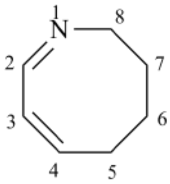
P-31.2.4.3 The use of the ‘dehydro’ prefix is not recommended to denote double bond unsaturation in heterocyclic rings having Hantzsch-Widman names. Names are formed preferably by using the ‘hydro’ prefix, as shown in the following examples.

Example:



(6*Z*,8*Z*)-2,3,4,5-tetrahydroazocine (PIN)

not



1,2,3,4-tetradehydroazocane

P-32 PREFIXES FOR SUBSTITUENT GROUPS DERIVED FROM PARENT HYDRIDES WITH A MODIFIED DEGREE OF HYDROGENATION

P-32.0 Introduction
P-32.1 Substituent groups derived from parent hydrides with ‘ene’ or ‘yne’ endings
P-32.2 Substituent groups modified by the prefix ‘hydro’
P-32.3 Retained names for substituent groups derived from unsaturated acyclic parent hydrides
P-32.4 Retained names for substituent groups derived from partially saturated polycyclic parent hydrides

P-32.0 INTRODUCTION

Names of substituents derived from the names of the corresponding unsaturated compounds described in Section P-31 are formed by using the appropriate suffixes ‘yl’, ‘ylidene’ or ‘ylidyne’, as described for the formation of substituent prefixes in Section P-29. These names of substituents may contain the endings ‘ene’ or ‘yne’, or the prefixes ‘hydro’ or ‘dehydro’ in the case of mancude compounds.

P-32.1 SUBSTITUENT GROUPS DERIVED FROM PARENT HYDRIDES WITH ‘ENE’ OR ‘YNE’ ENDINGS

P-32.1.1 Substituents derived from unsaturated acyclic compounds are named in two ways.

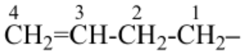
(1) As suffixes have priority for low locants, the position(s) of multiple bonds must be selected in accord with low locants assigned to free valences. These free valences can be in any position of modified parent structure(s). Accordingly, for acyclic parent structures, all locants for the free valences, including ‘1’, must be cited.

(2) Names can also be formed by substituting simple substituents into larger ones, in a manner similar to saturated prefixes described in Section P-29.

> A major change in the naming of substituents derived from unsaturated acyclic compounds is adopted in these recommendations. The longest chain is chosen as the parent chain in preference to the number or type of multiple bonds.

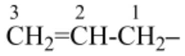
For the method used in the formation of preferred IUPAC names, see P-57.1.1.1.

Examples:



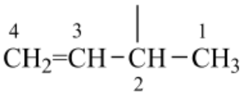
$\overset{4}{\mathrm{CH_2}}{=}\overset{3}{\mathrm{CH}}\text{-}\overset{2}{\mathrm{CH_2}}\text{-}\overset{1}{\mathrm{CH_2}}\text{–}$

(1) but-3-en-1-yl (preferred prefix)



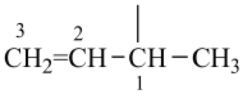
$\overset{3}{\mathrm{CH_2}}{=}\overset{2}{\mathrm{CH}}\text{-}\overset{1}{\mathrm{CH_2}}\text{–}$

(1) prop-2-en-1-yl (preferred prefix)



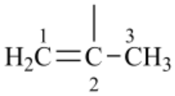
$\overset{4}{\mathrm{CH_2}}{=}\overset{3}{\mathrm{CH}}-\underset{2}{\overset{|}{\mathrm{CH}}}-\overset{1}{\mathrm{CH_3}}$

(1) but-3-en-2-yl (preferred prefix)



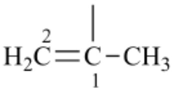
$\overset{3}{\mathrm{CH_2}}{=}\overset{2}{\mathrm{CH}}-\underset{1}{\overset{|}{\mathrm{CH}}}-\mathrm{CH_3}$

(2) 1-methylprop-2-en-1-yl



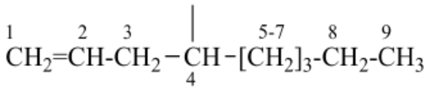
$\mathrm{H_2}\overset{1}{\mathrm{C}}{=}\underset{2}{\overset{|}{\mathrm{C}}}-\overset{3}{\mathrm{CH_3}}$

(1) prop-1-en-2-yl (preferred prefix)
isopropenyl (retained name,
but not substitutable, see P-32.3)



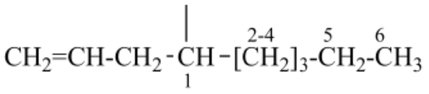
$\mathrm{H_2}\overset{2}{\mathrm{C}}{=}\underset{1}{\overset{|}{\mathrm{C}}}-\mathrm{CH_3}$

(2) 1-methylethen-1-yl



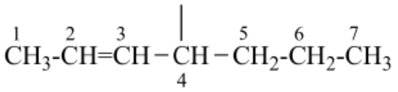
$\overset{1}{\mathrm{CH_2}}{=}\overset{2}{\mathrm{CH}}\text{-}\overset{3}{\mathrm{CH_2}}-\underset{4}{\overset{|}{\mathrm{CH}}}-\overset{5\text{-}7}{[\mathrm{CH_2}]_3}\text{-}\overset{8}{\mathrm{CH_2}}\text{-}\overset{9}{\mathrm{CH_3}}$

(1) non-1-en-4-yl (preferred prefix)



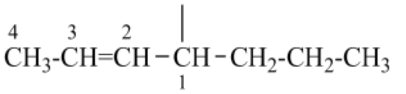
$\mathrm{CH_2{=}CH\text{-}CH_2}-\underset{1}{\overset{|}{\mathrm{CH}}}-\overset{2\text{-}4}{[\mathrm{CH_2}]_3}\text{-}\overset{5}{\mathrm{CH_2}}\text{-}\overset{6}{\mathrm{CH_3}}$

(2) 1-(prop-2-en-1-yl)hexyl
(not 1-pentylbut-3-en-1-yl)



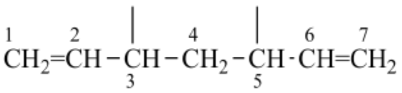
$\overset{1}{\mathrm{CH_3}}\text{-}\overset{2}{\mathrm{CH}}{=}\overset{3}{\mathrm{CH}}-\underset{4}{\overset{|}{\mathrm{CH}}}-\overset{5}{\mathrm{CH_2}}\text{-}\overset{6}{\mathrm{CH_2}}\text{-}\overset{7}{\mathrm{CH_3}}$

(1) hept-2-en-4-yl (preferred prefix)



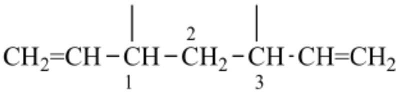
$\overset{4}{\mathrm{CH_3}}\text{-}\overset{3}{\mathrm{CH}}{=}\overset{2}{\mathrm{CH}}-\underset{1}{\overset{|}{\mathrm{CH}}}-\mathrm{CH_2\text{-}CH_2\text{-}CH_3}$

(2) 1-propylbut-2-en-1-yl



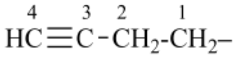
$\overset{1}{\mathrm{CH_2}}{=}\overset{2}{\mathrm{CH}}-\underset{3}{\overset{|}{\mathrm{CH}}}-\overset{4}{\mathrm{CH_2}}-\underset{5}{\overset{|}{\mathrm{CH}}}\cdot\overset{6}{\mathrm{CH}}{=}\overset{7}{\mathrm{CH_2}}$

(1) hepta-1,6-diene-3,5-diyl (preferred prefix)



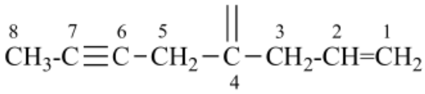
$\mathrm{CH_2{=}CH}-\underset{1}{\overset{|}{\mathrm{CH}}}-\overset{2}{\mathrm{CH_2}}-\underset{3}{\overset{|}{\mathrm{CH}}}\cdot\mathrm{CH{=}CH_2}$

(2) 1,3-diethenylpropane-1,3-diyl



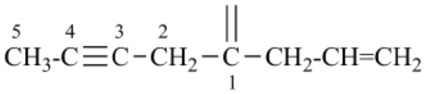
$\overset{4}{\mathrm{HC}}\equiv\overset{3}{\mathrm{C}}-\overset{2}{\mathrm{CH_2}}\text{-}\overset{1}{\mathrm{CH_2}}\text{–}$

(1) but-3-yn-1-yl (preferred prefix)



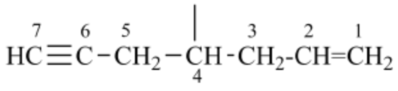
$\overset{8}{\mathrm{CH_3}}\text{-}\overset{7}{\mathrm{C}}\equiv\overset{6}{\mathrm{C}}-\overset{5}{\mathrm{CH_2}}-\underset{4}{\overset{\|}{\mathrm{C}}}-\overset{3}{\mathrm{CH_2}}\text{-}\overset{2}{\mathrm{CH}}{=}\overset{1}{\mathrm{CH_2}}$

(1) oct-1-en-6-yn-4-ylidene (preferred prefix)



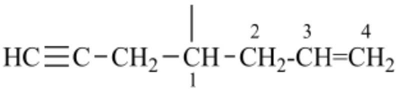
$\overset{5}{\mathrm{CH_3}}\text{-}\overset{4}{\mathrm{C}}\equiv\overset{3}{\mathrm{C}}-\overset{2}{\mathrm{CH_2}}-\underset{1}{\overset{\|}{\mathrm{C}}}-\mathrm{CH_2\text{-}CH{=}CH_2}$

(2) 1-(prop-2-en-1-yl)pent-3-yn-1-ylidene



$\overset{7}{\mathrm{HC}}\equiv\overset{6}{\mathrm{C}}-\overset{5}{\mathrm{CH_2}}-\underset{4}{\overset{|}{\mathrm{CH}}}\cdot\overset{3}{\mathrm{CH_2}}\text{-}\overset{2}{\mathrm{CH}}{=}\overset{1}{\mathrm{CH_2}}$

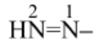
(1) hept-1-en-6-yn-4-yl (preferred prefix)



$\mathrm{HC}\equiv\mathrm{C}-\mathrm{CH_2}-\underset{1}{\overset{|}{\mathrm{CH}}}\cdot\overset{2}{\mathrm{CH_2}}\text{-}\overset{3}{\mathrm{CH}}{=}\overset{4}{\mathrm{CH_2}}$

(2) 1-(prop-2-yn-1-yl)but-3-en-1-yl

Note: In (1), lowest locants are assigned to the double bond; in (2) the principal chain includes the double bond.

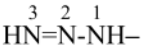


$$\overset{2}{H\text{N}}{=}\overset{1}{\text{N}}{-}$$

(1) diazenyl (preselected prefix; see P-12.2)

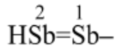
–N=N–

(1) diazenediyl (preselected prefix, see P-12.2)



$$\overset{3}{H\text{N}}{=}\overset{2}{\text{N}}{-}\overset{1}{\text{NH}}{-}$$

(1) triaz-2-en-1-yl (preselected prefix, see P-12.2)



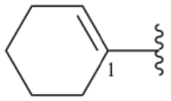
$$\overset{2}{H\text{Sb}}{=}\overset{1}{\text{Sb}}{-}$$

(1) distibenyl (preselected prefix; see P-12.2)

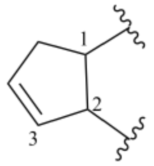
P-32.1.2 Monocyclic substituent groups

Method (1) described in P-32.1.1 is used to name monocyclic substituent groups.

Examples:



cyclohex-1-en-1-yl (preferred prefix)

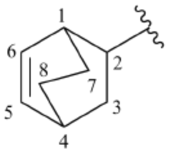


cyclopent-3-ene-1,2-diyl (preferred prefix)

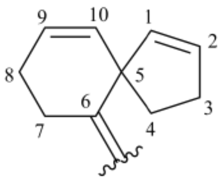
P-32.1.3 Substituent groups derived from parent hydrides having a fixed numbering

Lowest possible locants are assigned first to free valence(s), then to unsaturated sites, in accordance with the fixed numbering of the parent hydride.

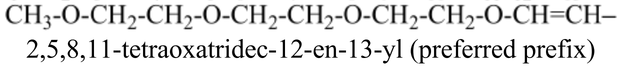
Examples:



bicyclo[2.2.2]oct-5-en-2-yl (preferred prefix)



spiro[4.5]deca-1,9-dien-6-ylidene (preferred prefix)



$$\overset{1}{CH_3}-\overset{2}{O}-\overset{3}{CH_2}-\overset{4}{CH_2}-\overset{5}{O}-\overset{6}{CH_2}-\overset{7}{CH_2}-\overset{8}{O}-\overset{9}{CH_2}-\overset{10}{CH_2}-\overset{11}{O}-\overset{12}{CH}=\overset{13}{CH}-$$

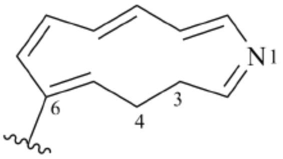
2,5,8,11-tetraoxatridec-12-en-13-yl (preferred prefix)
(not 3,6,9,12-tetraoxatridec-1-en-1-yl;
the suffix '-yl' is added to the parent hydride name 2,5,8,11-tetraoxatridecane)

P-32.2 SUBSTITUENT GROUPS DERIVED FROM PARENT HYDRIDES MODIFIED BY THE PREFIX 'HYDRO'

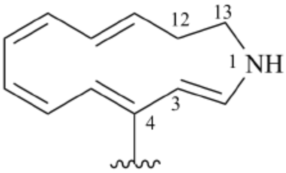
Names of partially unsaturated substituent groups derived from mancude compounds are formed by using the prefix 'hydro'. When a choice is possible, low locants are assigned in accord with the order of seniority (see P-44.2 and also P-59.1.10) for assigning lowest possible locants to several nomenclature features. Indicated and added indicated hydrogen atoms must be cited in names.

P-32.2.1 For heteromonocyclic parent hydrides, when there is a choice heteroatoms have the lower possible locants, then indicated hydrogen atoms, followed by free valence suffixes and finally 'hydro' prefixes.

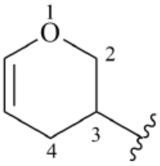
Examples:



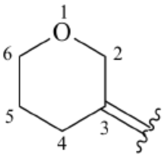
3,4-dihydro-1-aza[12]annulen-6-yl
1-azacyclododeca-1,5,7,9,11-pentaen-6-yl (preferred prefix)



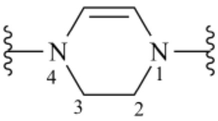
12,13-dihydro-1*H*-1-aza[13]annulen-4-yl
1-azacyclotrideca-2,4,6,8,10-pentaen-4-yl (preferred prefix)



3,4-dihydro-2*H*-pyran-3-yl
(preferred prefix)



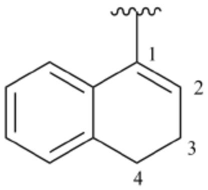
dihydro-2*H*-pyran-3(4*H*)-ylidene
oxan-3-ylidene (preferred prefix)



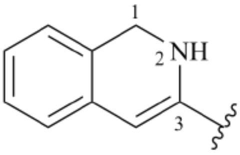
2,3-dihydropyrazine-1,4-diyl (preferred prefix)

P-32.2.2 For polycyclic mancude compounds, when there is a choice low locants go first to the fixed numbering of the system, then indicated hydrogen, followed by free valence suffix, and finally ‘hydro’ prefixes.

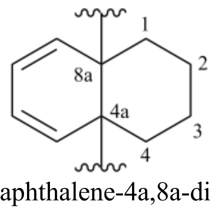
Examples:



3,4-dihydronaphthalen-1-yl (preferred prefix)



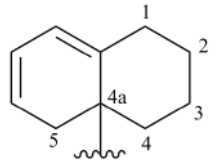
1,2-dihydroisoquinolin-3-yl (preferred prefix)



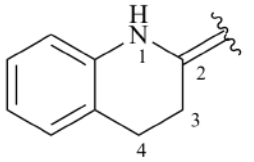
1,2,3,4-tetrahydronaphthalene-4a,8a-diyl (preferred prefix)

P-32.2.3 When the method of added indicated hydrogen (see P-58.2.2) is used and when a choice is possible, low locants are assigned in accordance with the fixed numbering of the system, then to indicated hydrogen, followed by free valence suffixes, ‘added indicated hydrogen’ atom, and finally to ‘hydro’ prefixes (see P-14.4).

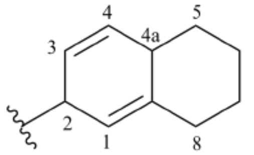
Examples:



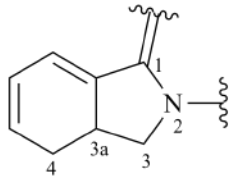
1,3,4,5-tetrahydronaphthalen-4a(2*H*)-yl (preferred prefix)



3,4-dihydroquinolin-2(1*H*)-ylidene (preferred prefix)



5,6,7,8-tetrahydronaphthalen-2(4a*H*)-ylidene (preferred prefix)



3a,4-dihydro-1*H*-isoindol-2(3*H*)-yl-1-ylidene (preferred prefix)

P-32.3 RETAINED NAMES FOR SUBSTITUENT GROUPS DERIVED FROM UNSATURATED ACYCLIC PARENT HYDRIDES

The names vinyl, for $CH_2=CH–$; vinylidene, for $CH_2=C=$; allyl, for $\overset{3}{C}H_2=\overset{2}{C}H\text{-}\overset{1}{C}H_2—$ allylidene, for $\overset{3}{C}H_2=\overset{2}{C}H\text{-}\overset{1}{C}H=$; and allylidyne, for $\overset{3}{C}H_2=\overset{2}{C}H\text{-}\overset{1}{C}\equiv$; are retained for general nomenclature only. Substitution is allowed, but not by alkyl or any other group that extends the carbon chain, or characteristic groups expressed by suffixes. The systematic names ethenyl, ethenylidene, prop-2-en-1-yl, prop-2-en-1-ylidene, and prop-2-en-1-ylidyne, respectively, are the preferred prefixes.

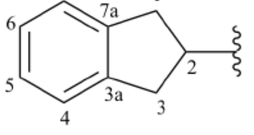
The name isopropenyl, for $CH_2=C(CH_3)–$, is a retained name but is not used as a preferred prefix. It is acceptable for general use, but substitution is not allowed. The preferred prefix is prop-1-en-2-yl.

The name styryl, for $C_6H_5\text{-}CH=CH–$, is a retained name used only in general nomenclature with substitution permitted only on the ring. The preferred prefix is 2-phenylethen-1-yl.

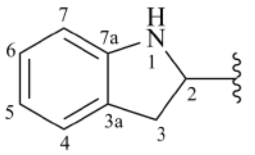
P-32.4 RETAINED NAMES FOR SUBSTITUENT GROUPS DERIVED FROM PARTIALLY SATURATED POLYCYCLIC PARENT HYDRIDES

The prefixes in Table 3.2 are retained but are acceptable only for general nomenclature and may be fully substituted; the preferred prefixes are formed systematically.

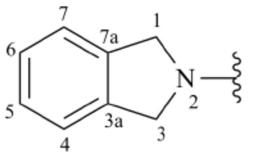
Table 3.2 Retained names of substituent groups for partially saturated polycyclic parent hydrides



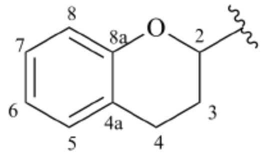
indan-2-yl (also 1-, 4- and 5-isomers)
2,3-dihydro-1*H*-inden-2-yl (preferred prefix) (also 1-, 4- and 5-isomers)



indolin-2-yl (also 1-, 3-, 4-, 5-, 6- and 7-isomers)
1,3-dihydro-2*H*-indol-2-yl (preferred prefix) (also 1-, 3-, 4-, 5-, 6- and 7-isomers)



isoindolin-2-yl (also 1-, 4- and 5-isomers)
2,3-dihydro-1*H*-isoindol-2-yl (preferred prefix) (also 1-, 4- and 5-isomers)

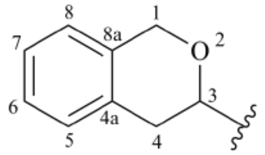


chroman-2-yl (also 3-, 4-, 5-, 6-, 7- and 8-isomers)
3,4-dihydro-2*H*-chromen-2-yl (also 3-, 4-, 5-, 6-, 7- and 8-isomers)
3,4-dihydro-2*H*-1-benzopyran-2-yl (also 3-, 4-, 5-, 6-, 7- and 8-isomers; preferred prefixes)

thiochroman-2-yl (S instead of O) (also 3-, 4-, 5-, 6-, 7- and 8-isomers)
3,4-dihydro-2*H*-thiochromen-2-yl (also 3-, 4-, 5-, 6-, 7- and 8-isomers)
3,4-dihydro-1-benzothiopyran-2-yl (also 3-, 4-, 5-, 6-, 7- and 8-isomers; preferred prefixes)

selenochroman-2-yl (Se instead of O) (also 3-, 4-, 5-, 6-, 7- and 8-isomers)
3,4-dihydro-2*H*-selenochromen-2-yl (also 3-, 4-, 5-, 6-, 7- and 8-isomers)
3,4-dihydro-2*H*-1-benzoselenopyran-2-yl (also 3-, 4-, 5-, 6-, 7- and 8-isomers; (preferred prefixes)

tellurochroman-2-yl (Te instead of O) (also 3-, 4-, 5-, 6-, 7- and 8-isomers)
3,4-dihydro-2*H*-tellurochromen-2-yl (also 3-, 4-, 5-, 6-, 7- and 8-isomers)
3,4-dihydro-2*H*-1-benzotelluropyran-2-yl (also 3-, 4-, 5-, 6-, 7- and 8-isomers; preferred prefixes)



isochroman-3-yl (also 1-, 4-, 5-, 6-, 7- and 8-isomers)
3,4-dihydro-1*H*-isochromen-3-yl (also 1-, 4-, 5-, 6-, 7- and 8-isomers)
3,4-dihydro-1*H*-2-benzopyran-3-yl (also 1-, 4-, 5-, 6-, 7- and 8-isomers; preferred prefixes)

isothiochroman-3-yl (S instead of O) (also 1-, 4-, 5-, 6-, 7- and 8-isomers)
3,4-dihydro-1*H*-isothiochromen-3-yl (also 1-, 4-, 5-, 6-, 7- and 8-isomers)
3,4-dihydro-1*H*-2-benzothiopyran-3-yl (also 1-, 4-, 5-, 6-, 7- and 8-isomers; preferred prefixes)

isoselenochroman-3-yl (Se instead of O) (also 1-, 4-, 5-, 6-, 7- and 8-isomers)
3,4-dihydro-1*H*-isoselenochromen-3-yl (also 1-, 4-, 5-, 6-, 7- and 8-isomers)
3,4-dihydro-1*H*-2-benzoselenopyran-3-yl (also 1-, 4-, 5-, 6-, 7- and 8-isomers; preferred prefixes)

isotellurochroman-3-yl (Te instead of O) (also 1-, 4-, 5-, 6-, 7- and 8-isomers)
3,4-dihydro-1*H*-isotellurochromen-3-yl (also 1-, 4-, 5-, 6-, 7- and 8-isomers)
3,4-dihydro-1*H*-2-benzotelluropyran-3-yl (also 1-, 4-, 5-, 6-, 7- and 8-isomers; preferred prefixes)

P-33 SUFFIXES

P-33.0 Introduction
P-33.1 Definitions
P-33.2 Functional suffixes
P-33.3 Cumulative suffixes

P-33.0 INTRODUCTION

This Section includes names of substituents denoting characteristic groups expressed as suffixes. These characteristic groups are essentially those having free valence(s) on atoms such as the chalcogens (O, S, Se, Te) and nitrogen. The concept is extended to carbon atoms linked to halogens, chalcogens and nitrogen, such as –CO-Cl, –CO-OH, –CS-SH, –

CHO, –CN. Radicals and ions are expressed by suffixes in substitutive nomenclature although they are not classified as characteristic groups.

P-33.1 DEFINITIONS

Suffixes are divided into ‘functional suffixes’ that express characteristic groups and ‘cumulative suffixes’ that are used to denote radicals and ions. Functional suffixes (P-33.2) are used to denote characteristic groups; they are exclusive because only one can be placed at the end of a name to represent the principal characteristic group or function. Suffixes designating radicals and ions, on the other hand, can be used in association with each other and also in association with functional suffixes (see Chapter P-7). In names, functional suffixes are always attached to the name of the parent hydride, modified or not by ‘ene’ and ‘yne’ endings. ‘Cumulative suffixes’ (see P-33.3) can be attached directly to the names of parent hydrides, modified or not by ‘ene’ and ‘yne’ endings; but when functional suffixes are present, cumulative suffixes are attached to them.

Examples:

CH_4 methane (PIN)	$\longrightarrow$	CH_5^+ methanium (PIN) (the suffix ‘-ium’ indicates addition of H^+)

P-33.2

CH_4 methane (PIN)	$\longrightarrow$	$CH_3\text{-}NH_2$ methanamine (PIN) (the suffix ‘-amine’ describes substitution)	$\longrightarrow$	$CH_3\text{-}NH_3^+$ methanaminium (PIN) (the suffix ‘-ium’ describes addition of H^+)
$CH_3\text{-}CH_3$ ethane (PIN)	$\longrightarrow$	$\bullet CH_2\text{-}CH_3$ ethyl (PIN; the suffix ‘-yl’ decribes the loss of one hydrogen atom)	$\longrightarrow$	$\bullet CH_2\text{-}CH^{2\bullet}$ ethan-1-yl-2-ylidene (PIN; the the suffix ‘-ylidene’ describes the loss of two hydrogen atoms)

FUNCTIONAL SUFFIXES

P-33.2.1 Basic functional suffixes

Basic suffixes are those composed only of oxygen and/or nitrogen, with or without association with carbon, as in the case of carboxylic acids, amides, nitriles and aldehydes, and also with sulfur to denote sulfonic acids and sulfinic acids, and the corresponding amides and hydrazides. They are listed in Table 3.3.

> The suffix ‘peroxol’, for –OOH, has been added to the list of basic suffixes. It is modified by functional replacement generating the suffixes ‘–*OS*-thioperoxol’ for –OSH, and ‘–*SO*-thioperoxol’ for –SOH. The suffix ‘sulfenic acid’, for –SOH, was abandoned in the 1993 Recommendations (ref. 2).

Table 3.3 Basic preferred and preselected suffixes, in decreasing order of seniority for citation as the principal characteristic group (preferred suffixes are those that contain a carbon atom)

	Formula	**Basic suffix**
(1)	–CO-OH	carboxylic acid (preferred suffix)
(2)	–(C)O-OH	oic acid (preferred suffix)
(3)	$–SO_2$-OH	sulfonic acid (preselected suffix)
(4)	–SO-OH	sulfinic acid (preselected suffix)
(5)	$–CO\text{-}NH_2$	carboxamide (preferred suffix)
(6)	$–(C)O\text{-}NH_2$	amide (preferred suffix)
(7)	$–CO\text{-}NHNH_2$	carbohydrazide (preferred suffix)
(8)	$–(C)O\text{-}NHNH_2$	hydrazide (preferred suffix)
(9)	–CN	carbonitrile (preferred suffix)
(10)	–(C)N	nitrile (preferred suffix)
(11)	–CHO	carbaldehyde (preferred suffix)
(12)	–(C)HO	al (preferred suffix)
(13)	=O	one (preselected suffix)
(14)	–OH	ol (preselected suffix)
(15)	–OOH	peroxol (preselected suffix)
(16)	$–NH_2$	amine (preselected suffix)

(17)	=NH	imine (preselected suffix)

P-33.2.2 Derived preferred and preselected suffixes

Derived suffixes are formed in various ways by modifying the basic suffixes of Table 3.3. There is no general rule governing the elision of the final letter ‘o’ of the functional replacement prefixes and infixes before a vowel. It is elided or not according to traditional usage, for example in the suffixes ‘thioic acid’ and ‘imidic acid’. The preferred suffixes are as follows:

(1) Basic suffixes that include a carbon atom are modified by functional replacement by using infixes to indicate the replacement of oxygen atoms by –OO–, –S–, =S, –Se–, =Se, –Te–, =Te, =NH and =NNH$_2$, as indicated in P-15.5; it is to be noted that the letter ‘x’ of ‘carboxylic’ is maintained before a vowel and that the letter ‘o’ is not elided before amide.

Examples:

–CO-OH	carboxylic acid (preferred suffix)
–C(O)-OOH	carboperoxoic acid (preferred suffix)
–C(O)-SH	carbothioic *S*-acid (preferred suffix)
–C(Se)-OH	carboselenoic *O*-acid (preferred suffix)
–C(=NH)-OH	carboximidic acid (preferred suffix)
–C(=NNH$_2$)-OH	carbohydrazonic acid (preferred suffix)
–C(=NH)-SH	carboximidothioic acid (preferred suffix)
–CO-NH$_2$	carboxamide (preferred suffix)
–C(Te)-NH$_2$	carbotelluroamide (preferred suffix)
–CO-NHNH$_2$	carbohydrazide (preferred suffix)
–C(S)-NHNH$_2$	carbothiohydrazide (preferred suffix)
–CHO	carbaldehyde (preferred suffix)
–CHS	carbothialdehyde (preferred suffix)

(2) Basic suffixes that include an implied carbon atom are modified by functional replacement, using prefixes to indicate the replacement of oxygen atoms by –OO–, –S–, =S, –Se–, =Se, –Te–, =Te, =NH and =NNH$_2$, as indicated in P-15.5; it is to be noted that the letter ‘o’ is not elided before amide and that an additional ‘o’ is elided from ‘imide’ before ‘oic’ for euphonic reasons.

Examples:

–(C)O-OH	oic acid (preferred suffix)
–(C)O-OOH	peroxoic acid (preferred suffix)
–(C)O-SH	thioic *S*-acid (preferred suffix)
–(C)Te-OH	telluroic *O*-acid (preferred suffix)
–(C)(=NH)-OH	imidic acid (preferred suffix) (not imidoic acid)
–(C)(=NNH$_2$)-OH	hydrazonic acid (preferred suffix)
–(C)(=NH)-SeH	imidoselenoic acid (preferred suffix)
–(C)O-NH$_2$	amide (preferred suffix)
–(C)S-NH$_2$	thioamide (preferred suffix)
–(C)O-NHNH$_2$	hydrazide (preferred suffix)
–(C)S-NHNH$_2$	thiohydrazide (preferred suffix)
–(C)HO	al (preferred suffix)
–(C)HSe	selenal (preferred suffix)

(3) Basic suffixes that do not include a carbon atom are modified by functional replacement nomenclature using prefixes to indicate the replacement of oxygen atoms by other chalcogen atoms.

Examples:

=O	one (preselected suffix)
=S	thione (preselected suffix)
=Se	selone (preselected suffix) (not selenone)
=Te	tellone (preselected suffix) (not tellurone)

$-OH$	ol (preselected suffix)
$-SH$	thiol (preselected suffix)
$-OOH$	peroxol (preselected suffix)
$-OSH$	*OS*-thioperoxol (preselected suffix)

(4) The stem ‘sulf’ is replaced by ‘selen’ and ‘tellur’ to generate the selenium and tellurium analogues of sulfonic and sulfinic acids.

Examples:

$-SO_2\text{-}OH$	sulfonic acid (preselected suffix)
$-SO\text{-}OH$	sulfinic acid (preselected suffix)
$-SeO_2\text{-}OH$	selenonic acid (preselected suffix)
$-TeO\text{-}OH$	tellurinic acid (preselected suffix)

(5) Suffixes of the type ‘sulfonic acid’ and analogues are modified by functional replacement by using infixes to indicate the replacement of oxygen atoms by $-OO-$, $-S-$, $=S$, $-Se-$, $=Se$, $-Te-$, $=Te$, $=NH$ and $=NNH_2$, as indicated in P-15.5.

Examples:

$-SO_2\text{-}OH$	sulfonic acid (preselected suffix)
$-SO_2\text{-}OOH$	sulfonoperoxoic acid (preselected suffix)
$-S(=NNH)_2\text{-}OH$	sulfonodihydrazonic acid (preselected suffix)
$-SeO\text{-}OH$	seleninic acid (preselected suffix)
$-SeO\text{-}SH$	seleninothioic *S*-acid (preselected suffix)
$-TeO_2\text{-}OH$	telluronic acid (preselected suffix)
$-Te(O)(=NH)\text{-}OH$	telluronimidic acid (preselected suffix)
$-SO\text{-}OH$	sulfinic acid (preselected suffix)
$-S(=NNH_2)\text{-}OH$	sulfinohydrazonic acid (preselected suffix)

(6) Names of amides and hydrazides are formed by replacing the ‘ic acid’ ending in suffixes by ‘amide’ or ‘hydrazide’, respectively ; a euphonic letter ‘o’ is added as required:

Examples:

$-(C)(=NH)\text{-}OH$	imidic acid (preferred suffix)
$-(C)(=NH)\text{-}NH_2$	imidamide (preferred suffix)
$-C(=NH)\text{-}OH$	carboximidic acid (preferred suffix)
$-C(=NH)\text{-}NH_2$	carboximidamide (preferred suffix)
$-(C)(=NNH_2)\text{-}OH$	hydrazonic acid (preferred suffix)
$-(C)(=NHNH_2)\text{-}NHNH_2$	hydrazonohydrazide (preferred suffix)
$-SO_2\text{-}OH$	sulfonic acid (preselected suffix)
$-SO_2\text{-}NH_2$	sulfonamide (preselected suffix)
$-SeO\text{-}OH$	seleninic acid (preselected suffix)
$-SeO\text{-}NHNH_2$	seleninohydrazide (preselected suffix)

(7) Suffixes with $-NH_2$ and $=NH$ groups substituted by an $-OH$ group are named in two ways:

(1) are named as *N*-hydroxy derivatives of amides or imidic acids;

(2) by modifying the ‘-oic acid’ or ‘-carboxylic acid’ suffix of a systematically named acid to ‘-hydroxamic acid’ or ‘-carbohydroxamic acid’ and ‘-hydroximic acid’ or ‘-carbohydroximic acid’, or the ‘-ic acid’ ending of the retained name of an acid to ‘-hydroxamic acid’ or ‘-hydroximic acid’. The letter ‘o’ is added for euphony between ‘h’ and a preceding consonant.

Method (1) is used for preferred IUPAC names.

Preferred IUPAC names are now named as *N*-hydroxy derivatives of amides or imidic acids.

Examples:

$CH_3\text{-}CH_2\text{-}CO\text{-}NH_2$
propanamide (PIN)

$\mathrm{CH_3\text{-}CH_2\text{-}CO\text{-}NH\text{-}OH}$
N-hydroxypropanamide (PIN)
propanohydroxamic acid

$\mathrm{CH_3\text{-}CH_2\text{-}C({=}NH)\text{-}OH}$
propanimidic acid (PIN)

$\mathrm{CH_3\text{-}CH_2\text{-}C({=}N\text{-}OH)\text{-}OH}$
N-hydroxypropanimidic acid (PIN)
propanohydroximic acid

P-33.3 CUMULATIVE SUFFIXES

Suffixes used to denote radical and ionic centers in a parent structure are given in Table 3.4. They are classified in decreasing order of seniority, radicals > anions > cations. Suffixes are added to the name of a parent hydride in the customary manner, or to suffixes expressing another type of radical or ion, or to suffixes denoting characteristic groups. Names of radicals are formed in the same manner as substituent groups (see P-29.2), with the exception that di- and trivalent radicals centered on a single atom are denoted by the suffixes 'ylidene' and 'ylidyne', respectively, and never by 'diyl' or 'triyl'.

Note: 'ene', 'yne', etc. are considered endings not suffixes; they are cumulative endings.

Table 3.4 Affixes for radical and ionic centers in parent structures

	Operation	**Suffix**	**Ending**
Radicals	Loss of H•	-yl	
	Loss of 2 H•		
	from one atom	-ylidene	
	from different atoms	-diyl	
	Loss of 3 H•		
	from one atom	-ylidyne	
	from different atoms	-triyl -ylylidene etc.	
Anions	Loss of H^+		
	Addition of H^-	-uide	ate, ite
Cations	Loss of H^-	-ylium	
	Addition of H^+	-ium	

Examples:

$\mathrm{CH_3\text{-}CH_3}$
ethane (PIN)

$\mathrm{CH_3\text{-}CH_2^{\bullet}}$
ethyl (PIN)

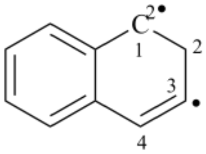
$\mathrm{{}^{-}\overset{2}{C}H_2\text{-}\overset{1}{C}H_2^{\bullet}}$
ethan-2-id-1-yl (PIN)

$\mathrm{CH_3\text{-}NH_2}$
methanamine (PIN)

$\mathrm{CH_3\text{-}NH_3^{+}}$
methanaminium (PIN)

$\mathrm{CH_3\text{-}\underset{\bullet}{\overset{+}{N}}H_2}$
methanaminiumyl (PIN)

$\mathrm{CH_3\text{-}NH^{\bullet}}$
methanaminyl (PIN)



naphthalen-3-yl-1(2*H*)-ylidene (PIN)

P-34 FUNCTIONAL PARENT COMPOUNDS

P-34.0 Introduction
P-34.1 Retained functional parent compounds
P-34.2 Substituent groups related to functional parent compounds

P-34.0 INTRODUCTION

Many trivial and semisystematic names have been used in organic chemistry. As systematic names have been increasingly recommended, the number of retained names (trivial and semisystematic) has been gradually reduced, in the 1979 Rules (ref. 1) and again in the 1993 Guide (ref. 2). Functional parent compounds have been defined and discussed in Section P-15.1.2 dealing with substitutive nomenclature. This subsection describes the 2005 codification of the list of functional parent compounds established in 1993 as far as their classification as preferred IUPAC names or names that are to be used only in general and specialized (see Chapter P-10) nomenclature is concerned.

Names recommended as preferred IUPAC names are described in the following section, P-34.1. Names that are recommended for general and specialized nomenclature are discussed in P-34.2, Chapter P-6, and Chapter P-10 along with systematic substitutive names recommended for the different classes of compounds.

P-34.1 RETAINED FUNCTIONAL PARENT COMPOUNDS

The retained names of the following functional parent compounds are used as preferred IUPAC names, as well as in general and specialized nomenclature. The lists in P-34.1.1 and P-34.1.2 are exhaustive for preferred IUPAC names; for more retained names of functional parent compounds recommended for use in general and specialized nomenclature, see P-34.1.3. The type of substitution (allowed or not) is specified for each compound in accordance with the general methodology indicated in P-15.1.8.

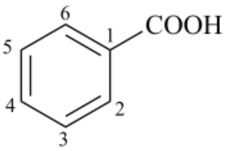
Inorganic functional parent compounds are acids and related compounds denoted by retained names that are preselected (see P-12.2); they are discussed in P-34.1.4.

P-34.1.1 Organic functional parent compounds (arranged by characteristic group class)
P-34.1.2 Organic functional parent compounds (arranged alphabetically)
P-34.1.3 Organic functional parent compounds for general and specialized nomenclature
P-34.1.4 Inorganic functional parent compounds

P-34.1.1 Organic functional parent compounds (arranged by characteristic group class)

P-34.1.1.1 Acids

CH_3-COOH
acetic acid (PIN)
(substitution allowed; see P-65.1.1.1)
ethanoic acid



benzoic acid (PIN)
(substitution allowed; see P-65.1.1.1)
benzenecarboxylic acid

H_2N-COOH
carbamic acid (PIN)
(substitution allowed; see P-65.2.1.1)
carbonamidic acid

HO-CO-OH
carbonic acid (PIN) (see P-65.2.1)

NC-OH
cyanic acid (PIN)
carbononitridic acid (see P-65.2.2)

H-COOH
formic acid (PIN)
(limited substitution see P-65.1.8)
methanoic acid

HOOC-COOH
oxalic acid (PIN)
(see P-65.1.1.1)
ethanedioic acid

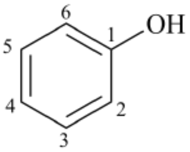
$H_2N\text{-CO-COOH}$
oxamic acid (PIN)
(substitution allowed; see P-65.1.6.1)
amino(oxo)acetic acid

$H_2N\text{-C(=NH)-OH}$
carbamimidic acid
(PIN; see P-65.2.1.3)
carbonamidimidic acid

P-34.1.1.2 Carbonyl compounds

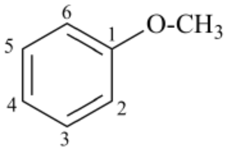
OHC-CHO
ethanedial (PIN)
glyoxal

P-34.1.1.3 Hydroxycompounds



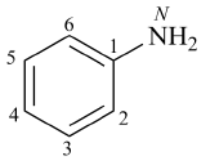
phenol (PIN)
(substitution allowed; P-63.1.1.1)
benzenol

P-34.1.1.4 Ethers



anisole (PIN)
(no substitution on anisole for PINs;
for general nomenclature substitution is permitted on the ring and on the α-methoxy group
only by groups listed in P-15.1.8.2.2; see also P-63.2.3)
methoxybenzene

P-34.1.1.5 Nitrogenous compounds

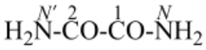


aniline (PIN);
(full substitution, see P-62.2.1.1.1)
benzenamine

$H_2\overset{5}{N}\text{-}\overset{4}{N}\text{=}\overset{3}{CH}\text{-}\overset{2}{N}\text{=}\overset{1}{N}H$
formazan (PIN)
(see P-68.3.1.3.5)
(diazenylmethylidene)hydrazine

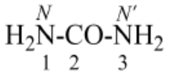
$H_2\overset{N}{N}\text{-C(=}\overset{N''}{N}\text{H)-}\overset{N'}{N}H_2$
guanidine (PIN)
(substitution allowed; see P-66.4.1.2.1)
carbonimidic diamide

$H_2N\text{-}OH$
hydroxylamine
(preselected name) (see P-68.3.1.1.1)



$H_2\overset{N'}{N}\text{-}\overset{2}{C}O\text{-}\overset{1}{C}O\text{-}\overset{N}{N}H_2$

oxamide (PIN)
(substitution allowed; see P-66.1.1.1.2.1)
oxalic diamide



$H_2\underset{1}{\overset{N}{N}}\text{-}\underset{2}{C}O\text{-}\underset{3}{\overset{N'}{N}}H_2$

urea (PIN)
(substitution allowed; see P-66.1.6.1.1)
carbonic diamide

P-34.1.2 Organic functional parent compounds (arranged alphabetically)

Retained name (PIN) or preselected name	**Alternative names**
acetic acid (substitution allowed; see P-65.1.1.1)	ethanoic acid
aniline (substitution allowed; see P-62.2.1.1.1)	benzenamine
anisole (no substitution on anisole for PINs; for general nomenclature substitution is permitted on the ring and on the α-methoxy group only by groups listed in P-15.1.8.2; see also P-63.2.3)	methoxybenzene
benzoic acid (substitution allowed; see P-65.1.1.1)	benzenecarboxylic acid
carbamic acid (substitution allowed; see P-65.2.1.1)	carbonimidic diamide
carbamimidic acid (substitution allowed; see P-65.2.1.3)	
carbonic acid (see P-65.2)	
cyanic acid (see P-65.2.2)	carbononitridic acid
formazan (substitution allowed; see P-68.3.1.3.5)	(hydrazinylidenemethyl)diazene (diazenylmethylidene)hydrazine
formic acid (limited substitution allowed; see P-65.1.8)	methanoic acid
guanidine (substitution allowed; see P-66.4.1.2.1)	carbonimidic diamide
hydroxylamine (special substitution; see P-68.3.1.1.1)	
oxamide (substitution allowed; see P-66.1.1.1.2)	oxalic diamide
oxamic acid (substitution allowed; see P-65.1.6.1)	
oxalic acid (see P-65.1.1.1)	ethanedioic acid
phenol (substitution allowed; see P-63.1.1.1)	benzenol
urea (substitution allowed; see P-66.1.6.1.1)	carbonic diamide

P-34.1.3 Organic functional parent compounds for general and specialized nomenclature

Functional parent compounds that were recommended in the 1979 recommendations (ref. 1) and /or the 1993 Guide (ref. 2) past can be used in general organic nomenclature. They are also used in biochemical nomenclature, the nomenclature of polymers, and in the nomenclature of natural products. Their formulae and names are described in Chapters P-6 and P-10. The different classes are: hydroxy compounds and ethers (see P-63), carbonyl compounds (see P-64), carboxylic acids (see P-65), amines (see P-62), sulfur compounds (see P-66.1.1.4.2) and sulfamic acid (see P-67.1.2.4.1.1), acyclic polynitrogen compounds (see P-66.1.6, P-68.3.1.3), and halogen compounds (see P-68.5).

Structures of alkaloids, steroids, terpenes, and similar compounds are given in Appendix 3.

P-34.1.4 Inorganic functional parent compounds

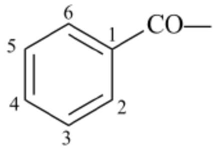
These compounds are described in P-67.1.1 and P-67.2.1.

P-34.2 SUBSTITUENT GROUPS RELATED TO FUNCTIONAL PARENT COMPOUNDS

P-34.2.1 Organic substituent groups (arranged by classes)

P-34.2.1.1 Acyl groups

$CH_3\text{-}CO–$
acetyl (preferred prefix)
(full substitution allowed except that the carbon chain cannot be extended see P-65.1.7.2.1)
ethanoyl
1-oxoethyl



benzoyl (preferred prefix)
(full substitution, see P-65.1.7.2.1)
benzenecarbonyl

H_2N-C(=NH)–
carbamimidoyl (preferred prefix)
(full substitution, see P-65.2.1.5)
C-aminocarbonimidoyl

H_2N-CO–
carbamoyl (preferred prefix)
(full substitution, see P-65.2.1.5)
aminocarbonyl

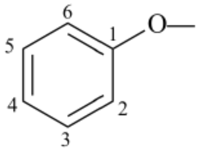
–CO–
carbonyl (preferred prefix)
(see P-65.2.1.5)

H_2N-CO-CO–
oxamoyl (preferred prefix)
(full substitution; see P-66.1.1.4.1.2)

H-CO–
formyl (preferred prefix)
(limited substitution; see P-65.1.7.2.1)
oxomethyl

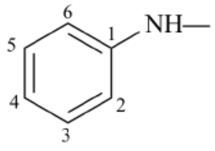
–CO-CO–
oxalyl (preferred prefix)
(see P-65.1.7.2.1)
ethanedioyl
dioxoethanediyl

P-34.2.1.2 Substituent groups derived from hydroxy compounds



phenoxy (preferred prefix)
(full substitution; see P-63.2.2.2)

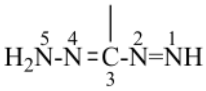
P-34.2.1.3 Nitrogenous substituent group names



anilino (preferred prefix)
(full substitution; see P-62.2.1.1.1)
phenylamino

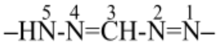
$\overset{5}{H_2N}\text{-}\overset{4}{N}\text{=}\overset{3}{C}H\text{-}\overset{2}{N}\text{=}\overset{1}{N}\text{—}$
formazan-1-yl (preferred prefix)
(full substitution; see P-68.3.1.3.5.2)
(hydrazinylidenemethyl)diazenyl

$\overset{1}{HN}\text{=}\overset{2}{N}\text{-}\overset{3}{C}H\text{=}\overset{4}{N}\text{-}\overset{5}{N}H\text{—}$
formazan-5-yl (preferred prefix)
(full substitution; see P-68.3.1.3.5.2)
(diazenylmethylidene)hydrazinyl



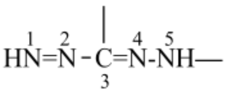
$$\mathrm{H_2\overset{5}{N}\text{-}\overset{4}{N}{=}\underset{3}{\overset{|}{C}}\text{-}\overset{2}{N}{=}\overset{1}{N}H}$$

formazan-3-yl (preferred prefix)
(full substitution; see P-68.3.1.3.5.2)
diazenyl(hydrazinylidene)methyl



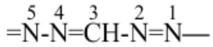
$$\mathrm{\text{–}H\overset{5}{N}\text{-}\overset{4}{N}{=}\overset{3}{C}H\text{-}\overset{2}{N}{=}\overset{1}{N}\text{–}}$$

formazan-1,5-diyl (preferred prefix)
(full substitution; see P-68.3.1.3.5.2)



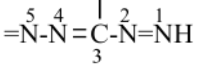
$$\mathrm{H\overset{1}{N}{=}\overset{2}{N}\text{-}\underset{3}{\overset{|}{C}}{=}\overset{4}{N}\text{-}\overset{5}{N}H\text{—}}$$

formazan-3,5-diyl (preferred prefix)
(full substitution; see P-68.3.1.3.5.2)



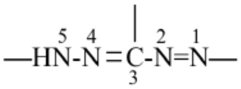
$$\mathrm{{=}\overset{5}{N}\text{-}\overset{4}{N}{=}\overset{3}{C}H\text{-}\overset{2}{N}{=}\overset{1}{N}\text{—}}$$

formazan-1-yl-5-ylidene (preferred prefix)
(full substitution; see P-68.3.1.3.5.2)



$$\mathrm{{=}\overset{5}{N}\text{-}\overset{4}{N}{=}\underset{3}{\overset{|}{C}}\text{-}\overset{2}{N}{=}\overset{1}{N}H}$$

formazan-3-yl-5-ylidene (preferred prefix)
(full substitution; see P-68.3.1.3.5.2)



$$\mathrm{\text{—}H\overset{5}{N}\text{-}\overset{4}{N}{=}\underset{3}{\overset{|}{C}}\text{-}\overset{2}{N}{=}\overset{1}{N}\text{—}}$$

formazan-1,3,5-triyl (preferred prefix)
(full substitution; see P-68.3.1.3.5.2)

$H_2N\text{-}C(=NH)\text{-}NH$—
carbamimidoylamino (preferred prefix)
(see P-66.4.1.2.1.3)
guanidino

$(H_2N)_2C=N$—
(diaminomethylidene)amino (preferred prefix)
(see P-66.4.1.2.1.3)

$H_2N\text{-}CO\text{-}CO\text{-}NH$—
oxamoylamino (preferred prefix)
(see P-66.1.1.4.5.1)

—HN-CO-NH—
oxalylbis(azanediyl) (preferred prefix)
(see P-66.1.1.4.5.2)

$H_2N\text{-}CO\text{-}NH$—
carbamoylamino (preferred prefix)
(see P-66.1.6.1.1.3)
(not ureido)

—HN-CO-NH—
carbonylbis(azanediyl) (preferred prefix)
(see P-66.1.6.1.1.3)

P-34.2.2 Organic substituent groups (arranged alphabetically)

Preferred Prefxes	**Alternative names**
acetyl (substitution allowed except that the carbon chain cannot be extended; see P-65.1.7.2.1)	ethanoyl
anilino (full substitution allowed; see P-62.2.1.1.1)	phenylamino
benzoyl (substitution allowed; see P-65.1.7.2.1)	benzenecarbonyl phenylcarbonyl
carbamimidoyl (substitution allowed; P-65.2.1.5)	*C*-aminocarbonimidoyl

carbamimidoylamino (see P-66.4.1.2.1.3)	
carbamoyl (substitution allowed; see P-65.2.1.5)	aminocarbonyl
carbamoylamino (see P-66.1.6.1.1.3)	
carbonyl (see P-65.2.1.5)	
carbonylbis(azanediyl) (see P-66.1.6.1.1.3)	
(diaminomethylidene)amino (see P-66.4.1.2.1.3)	
formazan-1,5-diyl (substitution allowed; P-68.3.1.3.5.2)	
formazan-3,5-diyl (substitution allowed; P-68.3.1.3.5.2)	
formazan-1,3,5-triyl (substitution allowed; see P-68.3.1.3.5.2)	
formazan-1-yl (substitution allowed; see P-68.3.1.3.5.2)	(hydrazinylidenemethyl)diazenyl
formazan-3-yl (substitution allowed; see P-68.3.1.3.5.2)	diazenyl(hydrazinylidene)methyl
formazan-5-yl (substitution allowed; see P-68.3.1.3.5.2)	(diazenylmethylidene)hydrazinyl
formazan-1-yl-5-ylidene (substitution allowed; see P-68.3.1.3.5.2)	
formazan-3-yl-5-ylidene (substitution allowed; see P-68.3.1.3.5.2)	
formyl (limited substitution allowed; see P-65.1.7.2.1)	methanoyl
oxamoylamino (see P-66.1.1.4.5.1)	
oxalylbis(azanediyl) (see P-66.1.1.4.5.2)	
oxamoyl (substitution allowed; see P-66.1.1.4.1.2)	
oxalyl (see P-65.1.7.2.1)	ethanedioyl
phenoxy (substitution allowed; see P-63.2.2.2)	phenyloxy

P-34.2.3 Substituent group names derived from organic compounds used in general and specialized nomenclature

These are discussed in Chapters P-6 and P-10.

P-34.2.4 Preselected substituent group names

Examples:

–NH-OH
hydroxyamino (preselected prefix)
(see P-68.3.1.1.1.5)

>N-OH
hydroxyazanediyl (preselected prefix)
(see P-68.3.1.1.1.5)

$-O-NH_2$
aminooxy (preselected prefix)
(see P-68.3.1.1.1.5)

P-35 PREFIXES CORRESPONDING TO CHARACTERISTIC GROUPS

P-35.0 Introduction
P-35.1 General methodology
P-35.2 Simple prefixes denoting characteristic groups
P-35.3 Compound substituent prefixes
P-35.4 Complex substituent prefixes
P-35.5 Mixed substituent prefixes

P-35.0 INTRODUCTION

Prefixes used to designate characteristic groups in substitutive nomenclature are those having free valence(s) attached to an atom of Group 17 (F, Cl, Br, and I) or Group 16 (O, S, Se, and Te), or to nitrogen. They have retained names or they are formed systematically by the methods described for substituent groups derived from parent hydrides (see P-29). Oxygen and nitrogen atoms can also be attached to a carbon atom, for example –CO-OH, $-CO-NH_2$, and $-CO-CH_2-CH_3$, or to a chalcogen atom, for example $-S(O)_2-OH$, $-Se(O)_2-OH$. These prefixes correspond to suffixes listed in P-33, for example the prefix ‘hydroxy’ for –OH corresponds to the suffix ‘ol’ for the same group. Prefixes are also derived from functional parents as defined in Sections P-34 and P-15.1.2, in particular acyl groups such as ‘acetyl’, for $-CO-CH_3$, derived from acetic acid, and phosphoryl, for –PO<.

Prefixes may have both a retained name and a systematic name only one of which can be a preferred IUPAC name. In order to facilitate the selection of preferred IUPAC names, clear indications are given in Chapter P-6 for each class of compounds. The prefixes are also alphabetically listed in Appendix 2, with indications concerning their status as preferred IUPAC names as well as their use in substitutive nomenclature and as functional replacement prefixes.

In this Section, the different types of prefixes used in substitutive nomenclature and in multiplicative nomenclature are described.

P-35.1 GENERAL METHODOLOGY

Substitutive prefixes corresponding to characteristic groups and functional parent compounds may be classified as simple (see P-29.1.1), compound (see P-29.1.2), and complex (see P-29.1.3); mixed substituent groups are complex substituent groups formed by the combination of substitutive and additive operations.

The multiple occurrence of simple prefixes is denoted by the basic numerical terms ‘di’, ‘tri’, etc., or by the derived prefixes ‘bis’, ‘tris’, ‘tetrakis’, etc., in order to distinguish between two simple prefixes and those including a basic multiplying term, for example disulfanyl, ‘–SSH’, and bis(sulfanyl), two –SH groups. Compound and mixed substituent prefixes require the derived multiplying terms ‘bis’, ‘tris’, ‘tetrakis’, etc., to designate their multiplicity in substitutive nomenclature.

Simple prefixes are either retained or systematically formed as follows:

(1) by subtracting hydrogen atom(s) from parent hydrides (described as substituent groups derived from parent hydrides in Section P-29), for example ‘sulfanyl’, –SH, and ‘diselanyl’, –SeSeH; from functional parent compounds, for example acetonyl, CH_3-CO-CH_2–; or from a contracted name, for example ‘methoxy’, CH_3-O–;

(2) acyl groups are formed by subtracting all −OH groups from oxoacids for example ‘acetyl’, CH_3-CO–, and ‘carbonyl’, >C=O.

P-35.2 SIMPLE PREFIXES DENOTING CHARACTERISTIC GROUPS

P-35.2.1 Retained traditional prefixes

–F
fluoro (preselected prefix)

–Cl
chloro (preselected prefix)

–Br
bromo (preselected prefix)

–I
iodo (preselected prefix)

–OH
hydroxy (preselected prefix)

=O
oxo (preselected prefix)

–O–
oxy (preselected prefix)

–COOH
carboxy (preferred prefix)

–SO_2-OH
sulfo (preselected prefix)
selenono (Se instead of S; preselected prefix)
tellurono (Te instead of S; preselected prefix)

–SO-OH
sulfino (preselected prefix)
selenino (Se instead of S; preselected prefix)
tellurino (Te instead of S; preselected prefix)

–NH_2
amino (preselected prefix)

–N_3
azido (preselected prefix)

=NH
imino (to the same atom; preselected prefix)

–N<
nitrilo (to different atoms; preselected prefix)

Note: In order to distinguish between HN= and –HN– (both are commonly called 'imino'), and between –N< and –N= (both are commonly called 'nitrilo'), systematic names based on the parent hydride azane are recommended for the latter in each pair.

$=N_2$
diazo (preselected prefix)

–NC
isocyano (preferred prefix)

–CN
cyano (preferred prefix)

–NCO
isocyanato (preferred prefix)
isothiocyanato (S instead of O; preferred prefix)
isoselenocyanato (Se instead of O; preferred prefix)
isotellurocyanato (Te instead of O; preferred prefix)

P-35.2.2 Substituents formed by subtracting one or more hydrogen atoms from mono- and dinuclear parent hydrides (see P-21.1, P-21.2).

Systematic names are formed by the general methodology described in P-29.3.1.

Examples:

–SH
sulfanyl (preselected prefix)
(not mercapto)

–S–
sulfanediyl (preselected prefix)
thio

=S
sulfanylidene (preselected prefix)
thioxo

–SS–
disulfanediyl (preselected prefix)
dithio

–SeH
selanyl (preselected prefix)
(not selenyl)

–Se–
selanediyl (preselected prefix)
seleno

=Se
selanylidene (preselected prefix)
selenoxo

–SeSe–
diselanediyl (preselected prefix)
diseleno

–TeH
tellanyl (preselected prefix)

–Te–
tellanediyl (preselected prefix)
telluro

=Te
tellanylidene (preselected prefix)
telluroxo

–TeTe–
ditellanediyl (preselected prefix)
ditelluro

H_2N-NH–
hydrazinyl (preslected prefix)
diazanyl

HN=N–
diazenyl (preselected prefix)

–NH–
azanediyl (preselected prefix) (to different atoms)

The systematic name based on the parent hydride azane is the preferred IUPAC name for –HN– in order to distinguish between HN= and –HN– both of which are commonly called 'imino'

–N=
azanylylidene (preselected prefix) (to different atoms)

≡N
azanylidyne (preselected prefix) (to the same atom)

The systematic name based on the parent hydride azane is the preferred IUPAC names for –N= in order to distinguish between –N< and –N= both of which are commonly called 'nitrilo'.

P-35.2.3 Simple prefixes derived from functional parent compounds

A few simple prefixes are derived from functional parent compounds described in P-34 and in P-67.

Examples:

–CO–
carbonyl (preferred prefix; see P-65.2.1.5)

–PO<
phosphoryl (preselected prefix; see P-67.1.4.1.1.2)

–SO_2–
sulfonyl (preselected prefix; see P-65.3.2.3)
sulfuryl

–SO–
sulfinyl (preselected prefix; see P-65.3.2.3)
thionyl

–SeO_2–
selenonyl (preselected prefix; see P-65.3.2.3)

–SeO–
seleninyl (preselected prefix; see P-65.3.2.3)

–TeO_2–
telluronyl (preselected prefix; see P-65.3.2.3)

–TeO–
tellurinyl (preselected prefix; see P-65.3.2.3)

CH_3-CO–
acetyl (preferred prefix; see P-65.1.7.2.1)

C_6H_5-CO–
benzoyl (preferred prefix; see P-65.1.7.2.1)

P-35.3 COMPOUND SUBSTITUENT PREFIXES

P-35.3.1 Names of compound prefixes derived from suffixes or functional parent compounds may be formed by substituting simple prefixes into other simple prefixes. When there is a choice, P-57.4 provides for the selection of a preferred compound prefix.

Examples:

–SSeH	selanylsulfanyl (preselected prefix)
–NH-Cl	chloroamino (preselected prefix)
$-NH-CH_3$	methylamino (preferred prefix)
–PH-Cl	chlorophosphanyl (preselected prefix)

P-35.3.2 Names of compound prefixes derived from suffixes or functional parent compounds may be formed by the additive operation called concatenation. This is used to assemble simple mono-, di-, tri-, and tetravalent prefixes. Hydrocarbyl divalent substituents can be attached to prefixes expressing characteristic groups. This method is used when no hydrogen atoms are present for substitution (see P-15.1); it is also used to form substituent groups in multiplicative nomenclature (see P-15.3.1.2.2)

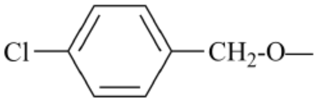
Examples:

$-O-CH_2-CH_2-CH_2-CH_2-CH_3$	pentyloxy (preferred prefix)
$-O-CH_2-C_6H_5$	benzyloxy (preferred prefix)
–CO-Cl	carbonochloridoyl (preferred prefix) chlorocarbonyl
–C(=NH)-OH	*C*-hydroxycarbonimidoyl (preferred prefix) hydroxy(imino)methyl
$-C(=N-NH_2)-OH$	*C*-hydroxycarbonohydrazonoyl (preferred prefix) hydrazinylidene(hydroxy)methyl
$-O-CH_2-CH_2-O-$	ethane-1,2-diylbis(oxy) (preferred prefix)
$>N-CH_2-N<$	methylenedinitrilo (preferred prefix)
$>P(S)-CH_2-P(S)<$	methylenebis(phosphorothioyl) (preferred prefix)

P-35.4 COMPLEX SUBSTITUENT PREFIXES

P-35.4.1 Names of complex substituent prefixes may be formed by substituting a simple or compound substituent prefix into a compound substituent prefix. When there is a choice, P-57.4 provides for the selection of a preferred complex substituent prefix.

Examples:

–NH-S-SeH	(selanylsulfanyl)amino (preselected prefix)
$-NH-CH_2Cl$	(chloromethyl)amino (preferred prefix)
	(4-chlorophenyl)methoxy (preferred prefix)
$-PH-NH-OCH_3$	(methoxyamino)phosphanyl (preferred prefix)

P-35.4.2 Names of complex substituent prefixes may be formed by adding simple or compound substituent prefixes to a compound substituent prefix by the process called ‘concatenation’.

Examples:

$-CO-O-CH_2-C_6H_5$	(benzyloxy)carbonyl (preferred prefix)
$-O-CS-OCH_3$	(methoxycarbonothioyl)oxy (preferred prefix)
$-CS-O-P(O)(OCH_3)_2$	[(dimethoxyphosphoryl)oxy]carbonothioyl (preferred prefix)

P-35.5 MIXED SUBSTITUENT PREFIXES

P-35.5.1 Mixed substituent prefix names are formed by combining the substitutive and additive operations.

Examples:

$CH_3-CH_2-O-SO-NH-$	(ethoxysulfinyl)amino (preferred prefix)
$CH_3-CO-S-CO-$	(acetylsulfanyl)carbonyl (preferred prefix)
$CH_3-CO-O-NH-SO-O-$	{[(acetyloxy)amino]sulfinyl}oxy (preferred prefix)
$(HS)_2(O)P-NH-$	[bis(sulfanyl)phosphoryl]amino (preselected prefix)

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Chapter P-4 RULES FOR NAME CONSTRUCTION

P-40 Introduction
P-41 Seniority order for classes
P-42 Seniority order for acids
P-43 Seniority order for suffixes
P-44 Seniority order for parent structures
P-45 Selection of the preferred IUPAC name
P-46 The principal chain in substituent groups

P-40 INTRODUCTION

In this Chapter, principles regarding name construction are presented. It is recognized that in chemical discussions it may sometimes be convenient to depart from rigorous rules in order to provide a name more appropriate to the chemical intent or to avoid obscuring an important feature. However, such deviations should not be done without good reason, and names so derived are not recommended for general use in publications.

The application of the principles and rules described in this Chapter has been devised to lead to a preferred IUPAC name. Preferred IUPAC names are not necessarily the aim of a practicing chemist who wants to communicate with his colleagues in familiar, well understood terms, but it may be appropriate to those who cite chemical names in legislative documents, in international trade and commerce, or for preparing programs for index purposes, databases, and retrieval systems.

This Chapter includes the general rules and orders of seniority used in substitutive nomenclature and in other types of nomenclature when required.

P-41 SENIORITY ORDER FOR CLASSES

The order of seniority of classes is given in Table 4.1. It ranks classes expressed by suffixes (classes 1 through 20) and classes based on the senior atom in compounds (classes 21 through 43). *

Table 4.1 General compound classes listed in decreasing order of seniority

1 Radicals

2 Radical anions

3 Radical cations

4 Anions

5 Zwitterions

6 Cations

7 Acids

7a 'Suffix' acids in the order carboxylic (not including carbonic or polycarbonic acids, which belong to sub-class '7b'), sulfonic, sulfinic, selenonic, seleninic, telluronic, tellurinic, each followed in turn by the corresponding peroxy, imidic, and hydrazonic acids. Chalcogen analogues follow each of the corresponding oxygen acids and, in each case, the chalcogen analogue with the greater number of the preferred chalcogen atom (O > S > Se > Te), considered first in −OOH groups, then in −OH groups as necessary. (See P-42 for the complete list of seniority of acids, P-43 for suffixes modified by functional replacement, and Table 4.4 for an extensive list of the order of seniority of all these suffixes.)

7b Carbon acids with no substitutable hydrogen atoms in the order polynuclear carbonic acids (tricarbonic acid, dicarbonic acid), then carbonic acid, and cyanic acid.

7c Oxoacids having substitutable hydrogen atoms attached to their central atoms and their acidic derivatives in the following decreasing order of seniority: azonic, azinic, phosphonic, phosphinic, phosphonous, phosphinous acids, etc. (see P-42 for the complete list).

7d Mononuclear and polynuclear oxoacids other than carbon acids without substitutable hydrogen atoms attached to their central atom (see 7b, above), but which may be functionalized or may form derivatives by functional replacement, which have substitutable hydrogen atoms.

7e Other monobasic ‘oxoacids’ used as functional parent compounds.

8 Anhydrides [substitutive nomenclature is used for cyclic anhydrides that are named as heterocycles (see 16 below); functional class names are given to acyclic anhydrides and to a few cyclic anhydrides corresponding to acids having retained names; cyclic anhydrides are preferred over noncyclic anhydrides, when functional names are used].

9 Esters (functional class names are given to noncyclic esters; lactones and other cyclic esters are named as heterocycles; see 16 below).

10 Acid halides and pseudohalides [first in the order of the corresponding acid given above, then in the order of the halogen atoms (–F > –Cl > –Br > –I); then in the following order of pseudohalogen groups ($–N_3$ > –CN > –NC > –NCO > –NCS > –NCSe > –NCTe > –CNO).

11 Amides [in the order of the corresponding acids; cyclic amides are named as heterocycles (see class 16 below)].

12 Hydrazides (in the order of the corresponding acids).

13 Imides (includes only cyclic imides derived from organic di- or polybasic acids having retained names).

14 Nitriles.

15 Aldehydes and chalcogen analogues.

16 Ketones (of the type –C-CO-C–), pseudoketones (of the type –C-CO-X , X-CO-X, or –CO-X-CO–, where X ≠ C, halogen, pseudohalogen, or NH_2, see P-64.1.2) and heterones (see P-64.4). See Classes 8, 9, 11 and 13, on lactones, lactams, anhydrides, imides.

17 Hydroxy compounds and chalcogen analogues (includes alcohols and phenols, which no longer have a separate ranking order).

18 Hydroperoxides (peroxols), i.e., –OOH.

19 Amines (defined as having three single covalent attachments to a nitrogen atom, i.e., NR_3).

20 Imines, R=NH or R=N-R′.

Classes denoted by the senior atom in heterane nomenclature

21 Nitrogen compounds: heterocycles, polyazanes, hydrazines (except for hydrazides), diazenes, hydroxylamines, azanes (except for amides, amines, and imines)

22 Phosphorus compounds: heterocycles, polyphosphanes, phosphanes

23 Arsenic compounds: heterocycles, polyarsanes, arsanes

24 Antimony compounds: heterocycles, polystibanes, stibanes

25 Bismuth compounds: heterocycles, polybismuthanes, bismuthanes

26 Silicon compounds: heterocycles, polysilanes, silanes

27 Germanium compounds: heterocycles, polygermanes, germanes

28 Tin compounds: heterocycles, polystannanes, stannanes

29 Lead compounds: heterocycles, polyplumbanes, plumbanes

30 Boron compounds: heterocycles, polyboranes, boranes

31 Aluminium compounds: heterocycles, polyalumanes, alumanes

32 Gallium compounds: heterocycles, polygallanes, gallanes

33 Indium compounds: heterocycles, polyindiganes, indiganes

34 Thallium compounds: heterocycles, polythallanes, thallanes

35 Oxygen compounds: heterocycles, polyoxidanes (trioxidane but not peroxides or ethers)

36 Sulfur compounds: heterocycles, polysulfanes (trisulfane, λ^6 and λ^4 mono and disulfanes, but not disulfides or sulfides)

37 Selenium compounds: heterocycles, polyselanes (triselane but not diselenides, selenides)

38 Tellurium compounds: heterocycles, polytellanes (tritellane but not ditellurides, tellurides)

39 λ^7, λ^5 and λ^3 halogen compounds in the order F > Cl > Br > I.

40 Carbon compounds: rings, chains

41 Ethers, then sulfides, sulfoxides, sulfones; then selenides, selenoxides, etc.

42 Peroxides, then chalcogen analogues with the greater number of the senior chalcogen atom, where O > S > Se > Te.

43 λ^1 Halogen compounds in the order F > Cl > Br > I

* In this table, the symbol ‘>’ means ‘is senior to’.

Examples:

$HOOC-CH_2-CH_2-$
2-carboxyethyl (preferred prefix)
[free valence = radical > carboxylic acid]

$(CH_3)_3N^+-CH_2-COO^-$
(*N*,*N*-dimethylmethanaminiumyl)acetate (PIN)
(anion > cation)

$HO-CH_2-CH_2-CONH_2$
3-hydroxypropanamide (PIN)
(amide > alcohol)

$OHC-CH_2-CH_2-CN$
4-oxobutanenitrile (PIN)
(nitrile > aldehyde)

$HSSS-SiH_3$
trisulfanylsilane
(preselected name; see P-12.2) (Si > S)

BH_2-PH_2
boranylphosphane
(preselected name; see P-12.2) (P > B)

$(CH_3)_4Si$
tetramethylsilane (PIN)
(Si > C)

$(C_6H_5)_3P$
triphenylphosphane (PIN)
(P > C)

$CH_3-O-CH_2-S-CH_3$
methoxy(methylsulfanyl)methane (PIN)
(C > ether and sulfide)

$CH_3-SeSe-CH_2-S-CH_3$
(methyldiselanyl)(methylsulfanyl)methane (PIN)
(C > diselenide and sulfide)

$CH_3-S-CH_2-CH_2-SO-CH_3$
1-(methanesulfinyl)-2-(methylsulfanyl)ethane (PIN)
(C > sulfide and sulfoxide)

P-42 SENIORITY ORDER FOR ACIDS

Acids of class 7 (see Table 4.1) in the order of classes of compounds are further classified into subclasses. These correspond to acids expressed by suffixes and acids used as functional parents (see P-34). The following subsections complete the brief description given in Class 7; the acids are described in decreasing seniority order.

P-42.1 Class 7a. Acids expressed by suffixes (excludes carbonic and polycarbonic acids)
P-42.2 Class 7b. Carbon acids with no substitutable hydrogen atoms
P-42.3 Class 7c. Noncarbon acids having substitutable hydrogen atoms on the central atom
P-42.4 Class 7d. Noncarbon acids used to generate derivatives having substitutable hydrogen atoms
P-42.5 Class 7e. Other monobasic ‘oxo’ acids used as functional parents.

P-42.1 CLASS 7a. ACIDS EXPRESSED BY SUFFIXES (EXCLUDES CARBONIC AND POLYCARBONIC ACIDS)

carboxylic acids	$-COOH$	-carboxylic acid
	$-(C)O-OH$	-oic acid
sulfonic acids	$-SO_2-OH$	-sulfonic acid
sulfinic acids	$-SO-OH$	-sulfinic acid
selenonic acids	$-SeO_2-OH$	-selenonic acid
seleninic acids	$-SeO-OH$	-seleninic acid
telluronic acids	$-TeO_2-OH$	-telluronic acid
tellurinic acids	$-TeO-OH$	-tellurinic acid

P-42.2 CLASS 7b. CARBON ACIDS WITH NO SUBSTITUTABLE HYDROGEN ATOMS

polycarbonic acids

dicarbonic acid

carbonic acid

cyanic acid

P-42.3 CLASS 7c. NONCARBON ACIDS HAVING SUBSTITUTABLE HYDROGEN ATOMS ON THE CENTRAL ATOM

All these names are preselected names. In this class, criteria for seniority are, in descending order:

(a) the central atom first in the list N > P > As > Sb > B;
(b) maximum number of central atoms;
(c) homopolyacids (isopolyacids) (see ref. 12);
(d) having contiguous central atoms;
(e) maximum number of acidic (–OH) groups;
(f) highest oxidation number for the central atom

For consistency in the names of polynuclear oxoacids, the numerical infix ‘di’ has been uniformly used in naming dinuclear ‘hypo’ acids, for example hypodiphosphorous acid, rather than hypophosphorous acid.

azonic acid	$NH(O)(OH)_2$
azinic acid	$NH_2(O)(OH)$
polyphosphonic acids	$(HO)PH(O)\text{-}O\text{-}[PH(O)\text{-}O\text{-}]_n PH(O)(OH)$
diphosphonic acid	$(HO)PH(O)\text{-}O\text{-}PH(O)(OH)$
hypodiphosphonic acid (for the prefix ‘hypodi’ see P-67.2.1)	$(HO)(O)HP\text{-}PH(O)(OH)$
phosphonic acid	$PH(O)(OH)_2$
polyphosphonous acids	$(HO)PH\text{-}O\text{-}[PH\text{-}O\text{-}]_n PH(OH)$
diphosphonous acid	$(HO)PH\text{-}O\text{-}PH(OH)$
hypodiphosphonous acid (for the prefix ‘hypodi’ see P-67.2.1)	$(HO)HP\text{-}PH(OH)$
phosphonous acid	$PH(OH)_2$
phosphinic acid	$PH_2(O)(OH)$
phosphinous acid	$PH_2(OH)$
polyarsonic acids > diarsonic acid > hypodiarsonic acid (for the prefix ‘hypodi’ see P-67.2.1)	
arsonic acid	$AsH(O)(OH)_2$
polyarsonous acids > diarsonous acid > hypodiarsonous acid (for the prefix ‘hypodi’ see P-67.2.1)	
arsonous acid	$AsH(OH)_2$
arsinic acid	$AsH_2(O)(OH)$
arsinous acid	$AsH_2(OH)$
polystibonic acids > distibonic acid > hypodistibonic acid (for the prefix ‘hypodi’ see P-67.2.1)	
stibonic acid	$SbH(O)(OH)_2$
polystibonous acids > distibonous acid > hypodistibonous acid (for the prefix ‘hypodi’ see P-67.2.1)	
stibonous acid	$SbH(OH)_2$
stibinic acid	$SbH_2(O)(OH)$
stibinous acid	$SbH_2(OH)$
diboronic acid	$(HO)BH\text{-}O\text{-}BH(OH)$
hypodiboronic acid (for the prefix ‘hypodi’ see P-67.2.1)	$(HO)HB\text{-}BH(OH)$
boronic acid	$BH(OH)_2$
borinic acid	$BH_2(OH)$

P-42.4 CLASS 7d. NONCARBON ACIDS USED TO GENERATE DERIVATIVES HAVING SUBSTITUTABLE HYDROGEN ATOMS

All these names are preselected names.

In this class, criteria for seniority are, in descending order:

(a) the central atom first in the list: P > As > Sb > Si > B > S > Se >Te;
(b) maximum number of central atoms;
(c) homopolyacids (isopolyacids) (see ref. 12);
(d) polyacids having contiguous central atoms;
(e) maximum number of acidic groups (-OH groups);
(f) highest oxidation number for the central atom.

polyphosphoric acids	$(HO)_2P(O)\text{-}O\text{-}[PO(OH)\text{-}O\text{-}]_nP(O)(OH)_2$
polyphosphorous acids	$(HO)_2P\text{-}O\text{-}[P(OH)\text{-}O\text{-}]_n\text{-}P(OH)_2$
tetraphosphoric acid	$(HO)_2P(O)\text{-}O\text{-}P(O)(OH)\text{-}O\text{-}P(O)(OH)\text{-}O\text{-}P(O)(OH)_2$
triphosphoric acid	$(HO)_2P(O)\text{-}O\text{-}P(O)(OH)\text{-}O\text{-}P(O)(OH)_2$
diphosphoric acid	$(HO)_2P(O)\text{-}O\text{-}P(O)(OH)_2$
diphosphorous acid	$(HO)_2P\text{-}O\text{-}P(OH)_2$
hypodiphosphoric acid (for the prefix ‘hypodi’ see P-67.2.1)	$(HO)_2(O)P\text{-}P(O)(OH)_2$
hypodiphosphorous acid (for the prefix ‘hypodi’ see P-67.2.1)	$(HO)_2P\text{-}P(OH)_2$
phosphoric acid	$P(O)(OH)_3$
phosphorous acid	$P(OH)_3$
polyarsoric acids > polyarsorous acids > diarsoric acid > diarsorous acid > hypodiarsoric acid > hypodiarsorous acid (for the prefix ‘hypodi’ see P-67.2.1)	
arsoric acid	$As(O)(OH)_3$
arsorous acid	$As(OH)_3$
polystiboric acids > polystiborous acid > distiboric acid > distiborous acid > hypodistiboric acid > hypodistiborous acid (for the prefix ‘hypodi’ see P-67.2.1)	
stiboric acid	$Sb(O)(OH)_3$
stiborous acid	$Sb(OH)_3$
silicic acid	$Si(OH)_4$
(formerly orthosilicic acid. See P-67.1.1.1, P-67.1.2.2 and Table IR-8.1, ref. 12.)	
diboric acid	$(HO)_2B\text{-}O\text{-}B(OH)_2$
hypodiboric acid (for the prefix ‘hypodi’ see P-67.2.1)	$(HO)_2B\text{-}B(OH)_2$
boric acid	$B(OH)_3$
polysulfuric acids	$(HO)SO_2\text{-}O\text{-}[SO_2\text{-}O\text{-}]_nSO_2(OH)$
polysulfurous acids	$(HO)SO\text{-}O\text{-}[SO\text{-}O\text{-}]_nSO(OH)$
disulfuric acid	$(HO)SO_2\text{-}O\text{-}SO_2(OH)$
disulfurous acid (ambiguous see P-67.3.2)	$(HO)S(O)\text{-}O\text{-}S(O)(OH)$
dithionic acid (hypodisulfuric acid) (for the prefix ‘hypodi’ see P-67.2.1)	$(HO)O_2S\text{-}SO_2(OH)$
dithionous acid (hypodisulfurous acid)	$(HO)(O)S\text{-}S(O)(OH)$
sulfuric acid	$S(O)_2(OH)_2$
sulfurous acid	$S(O)(OH)_2$
polyselenic acids > polyselenous acids > diselenic acid > diselenous acid > hypodiselenic acid > hypodiselenous acid (for the prefix ‘hypodi’ see P-67.2.1)	
selenic acid	$Se(O)_2(OH)_2$
selenous acid	$Se(O)(OH)_2$
polytelluric acids > polytellurous acids > ditelluric acid > ditellurous acid > hypoditelluric acid > hypoditellurous acid (for the prefix ‘hypodi’ see P-67.2.1)	
telluric acid	$Te(O)_2(OH)_2$
tellurous acid	$Te(O)(OH)_2$

P-42.5 CLASS 7e. OTHER MONOBASIC ‘OXO’ ACIDS USED AS FUNCTIONAL PARENTS

All these names are preselected names. In this class, criteria for seniority are, in descending order:

(a) the central atom first in the list N > F > Cl > Br > I;

(b) highest oxidation number for the central atom.

nitric acid	$HO\text{-}NO_2$
nitrous acid	HO-NO
perfluoric acid	$F(O)_3OH$
fluoric acid	$F(O)_2OH$
fluorous acid	F(O)OH
hypofluorous acid	FOH
perchloric acid	$Cl(O)_3OH$
chloric acid	$Cl(O)_2OH$
chlorous acid	Cl(O)OH
hypochlorous acid	ClOH
perbromic acid	$Br(O)_3OH$
bromic acid	$Br(O)_2OH$
bromous acid	Br(O)OH
hypobromous acid	BrOH
periodic acid	$I(O)_3OH$
iodic acid	$I(O)_2OH$
iodous acid	I(O)OH
hypoiodous acid	IOH

P-43 SENIORITY ORDER FOR SUFFIXES

P-43.0 Introduction
P-43.1 General methodology of functional replacement

P-43.0 INTRODUCTION

Suffixes are modified as indicated in Table 4.3 for acids and in Table 4.4 for all substituent suffixes. The order of seniority for suffixes is described in this Section. It is based on the seniority of classes 7 through 20 given in Table 4.1 and includes suffixes modified by functional replacement.

P-43.1 GENERAL METHODOLOGY OF FUNCTIONAL REPLACEMENT

Suffixes are modified as indicated in Table 4.3 for acids and in Table 4.4 for acids and other classes. Prefixes and infixes are used as indicated in Table 4.2. Prefixes are used to modify suffixes such as ‘ol’, ‘al’, for example ‘thiol’ and ‘thial’. Infixes are recommended to modify the suffixes ‘carboxylic acid’, ‘sulfonic acid’, and related suffixes, for example ‘carboperoxoic acid’ and ‘sulfonothioic acid’.

Table 4.2 Prefixes and infixes, in decreasing order of seniority, used to generate suffixes in preferred IUPAC names by functional replacement

Prefix	Infix	Replaced atom(s)	Replacing atom(s)
peroxy-	-peroxo-	–O–	–OO–
thioperoxy-	-(thioperoxo)-	–O–	–OS– or –SO–
dithioperoxy-	-(dithioperoxo)-	–O–	–SS–
thio-	-thio-	–O– or =O	–S– or =S
seleno-	-seleno-	–O– or =O	–Se– or =Se
telluro-	-telluro-	–O– or =O	–Te– or =Te
imido-	-imido-	=O	=NH
hydrazono-	-hydrazono-	=O	$=NNH_2$

When several oxygen atoms are replaceable, the following criteria are applied, in order, until a decision is reached:

(a) maximum number of oxygen atoms, then S, Se, and Te atoms, =NH and =NNH_2 groups;
(b) maximum number of oxygen atoms, then S, Se, and Te atoms, in −OO− groups;
(c) oxygen atoms, then S, Se, and Te atoms, in −(O)OH and −OH groups.

The order of seniority is described, in the case of carboxylic acids, sulfonic acids and sulfinic acids, by indicating, after the name of the modified suffix the number and kind of atoms used in the replacement operation (see Table 4.3).

Table 4.3 gives the list, in decreasing order, of the seniority of suffixes and suffixes modified by functional replacement for carboxylic and sulfonic acids. Sulfinic acid suffixes are similar to sulfonic acids. Selenium and tellurium acid suffixes are formed by replacing ‘sulf’ by ‘selen’ or ‘tellur’.

Table 4.3 Carboxylic and sulfonic acid suffixes generated for IUPAC preferred names by functional replacement, in decreasing order of seniority

1. Carboxylic acids

–COOH	carboxylic acid	
–CO-OOH	carboperoxoic acid	(3O)
–CS-OOH	carboperoxothioic *OO*-acid	(2O,1S; OO)
–CSe-OOH	carboperoxoselenoic acid	(2O,1Se; OO)
–CO-SOH	carbo(thioperoxoic) *SO*-acid	(2O,1S; OS; OH)
–CO-OSH	carbo(thioperoxoic) *OS*-acid	(2O,1S; OS; SH)
–CO-SeOH	carbo(selenoperoxoic) *SeO*-acid	(2O,1Se; OSe; OH)
–CO-OSeH	carbo(selenoperoxoic) *O*Se-acid	(2O,1Se; OSe; SeH)
–CS-SOH	carbothio(thioperoxoic) *SO*-acid	(1O,2S; OS; OH)
–CS-OSH	carbothio(thioperoxoic) *OS*-acid	(1O,2S; OS; SH)
–CSe-OSH	carboseleno(thioperoxoic) *OS*-acid	(1O,1S,1Se;OS; SH)
–CS-SeOH	carbo(selenoperoxo)thioic *SeO*-acid	(1O,1S,1Se;OSe: OH)
–CS-OSeH	carbo(selenoperoxo)thioic *OSe*-acid	(1O,1S,1Se; OSe; SeH)
–CS-SSH	carbo(dithioperoxo)thioic acid	(3S)
–CSe-SeSeH	carbo(diselenoperoxo)selenoic acid	(3Se)
–CTe-TeTeH	carbo(ditelluroperoxo)telluroic acid	(3Te)
–CS-OH	carbothioic *O*-acid	(1O,1S; OH)
–CO-SH	carbothioic *S*-acid	(1O,1S; SH)
–CS-SH	carbodithioic acid	(2S)
–CSe-SH	carboselenothioic *S*-acid	(1S,1Se; SH)
–CS-SeH	carboselenothioic *Se*-acid	(1S,1Se; SeH)
–CSe-SeH	carbodiselenoic acid	(2Se)
–CTe-SeH	carboselenotelluroic *Se*-acid	(1Se,1Te; SeH)
–CTe-TeH	carboditelluroic acid	(2Te)
–C(=NH)-OH	carboximidic acid	
–C(=NH)-OOH	carboximidoperoxoic acid	(2O,1N; OO)
–C(=NH)-SOH	carboximido(thioperoxoic) *SO*-acid	(1O,1S,1N; OS; OH)
–C(=NH)-OSH	carboximido(thioperoxoic) *OS*-acid	(1O,1S,1N; OS; SH)
–C(=NH)-SSH	carbo(dithioperoxo)imidic acid	(2S,1N; SS)
–C(=NH)-SeSH	carboximido(selenothioperoxoic) *SeS*-acid	(1S,1Se,1N; SSe; SH)
–C(=NH)-SH	carboximidothioic acid	(1S,1N)
–C(=NH)-SeH	carboximidoselenoic acid	(1Se,1N)
–C(=NH)-TeH	carboximidotelluroic acid	(1Te,1N)
–C(=NNH_2)-OH	carbohydrazonic acid	
–C(=NNH_2)-OOH	carbohydrazonoperoxoic acid	(2O,1NN; OO)
–C(=NNH_2)-SOH	carbohydrazono(thioperoxoic) *SO*-acid	(1O,1S,1NN; OS; OH)
–C(=NNH_2)-OSH	carbohydrazono(thioperoxoic) *OS*-acid	(1O,1S,1NN; OS; SH)
–C(=NNH_2)-TeTeH	carbo(ditelluroperoxo)hydrazonic acid	(2Te,1NN; TeTe)

2. Sulfonic acids

–SO_2-OH	sulfonic acid	
–SO_2-OOH	sulfonoperoxoic acid	(4O)

–S(O)(S)-OOH	sulfonoperoxothioic *OO-acid*	(3O,1S; OO)
–S(O)(Se)-OOH	sulfonoperoxoselenoic *OO*-acid	(3O,1Se; OO)
–SO_2-SOH	sulfono(thioperoxoic) *SO*-acid	(3O,1S; OS; OH)
–SO_2-OSH	sulfono(thioperoxoic) *OS*-acid	(3O,1S; OS; SH)
–SS_2-OOH	sulfonoperoxodithioic *OO*-acid	(2O,2S; OO)
–S(O)(S)-SOH	sulfonothio(thioperoxoic) *SO*-acid	(2O,2S; OS; OH)
–S(S)(Se)-OOH	sulfonoperoxoselenothioic *OO*-acid	(2O,1S,1Se; OO)
–SSeSe-SSH	sulfono(dithioperoxo)diselenoic acid	(2S,2Se; SS)
–SS_2-SeSeH	sulfono(diselenoperoxo)dithioic acid	(2S,2Se; SeSe)
–STe_2-TeTeH	sulfono(ditelluroperoxo)ditelluroic acid	(4Te)
–S(O)(S)-OH	sulfonothioic *O*-acid	(2O,1S; OH)
–SO_2-SH	sulfonothioic *S*-acid	(2O,1S; SH)
–SO_2-SeH	sulfonoselenoic *Se*-acid	(2O,1Se; SeH)
–SS_2-OH	sulfonodithioic *O*-acid	(1O,2S; OH)
–S(O)(S)-SH	sulfonodithioic *S*-acid	(1O,2S; SH)
–S(Se)(Te)-OH	sulfonoselenotelluroic *O*-acid	(1O,1Se,1Te; OH)
–S(O)(Te)-SeH	sulfonoselenotelluroic *Se*-acid	(1O,1Se,1Te; SeH)
–S(O)(Se)-TeH	sulfonoselenotelluroic *Te*-acid	(1O,1Se.1Te; TeH)
–S(S_2)-SH	sulfonotrithioic acid	(3S)
–S(O)(=NH)-OH	sulfonimidic acid	
–S(O)(=NH)-OOH	sulfonimidoperoxoic acid	(3O,1N; OO)
–S(S)(=NH)-OOH	sulfonimidoperoxothioic *OO*-acid	(2O,1S,1N; OO; OH)
–S(O)(=NH)-SOH	sulfonimido(thioperoxoic) *SO*-acid	(2O,1S,1N; OS; OH)
–S(O)(=NH)-OSH	sulfonimido(thioperoxoic) *OS*-acid	(2O,1S,1N; OS; SH)
–S(S)(=NH)-OH	sulfonimidothioic *O*-acid	(1O,1S; OH)
–S(O)(=NH)-SH	sulfonimidothioic *S*-acid	(1O,1S; SH)
–S(S)(=NH)-SH	sulfonimidodithioic acid	(2S)
–S(Se)(=NH)-SH	sulfonimidoselenothioic *S*-acid	(1S,1Se; SH)
–S(S)(=NH)-SeH	sulfonimidoselenothioic *Se*-acid	(1S,1Se; SeH)
–S(Te)(=NH)-TeH	sulfonimidoditelluroic acid	(2Te)
–$S(=NH)_2$-OH	sulfonodiimidic acid	
–$S(=NH)_2$-OOH	sulfonodiimidoperoxoic acid	(2O,2N; OO)
–$S(=NH)_2$-SOH	sulfonodiimido(thioperoxoic) *SO*-acid	(1O,1S,2N: OS; OH)
–$S(=NH)_2$-OSH	sulfonodiimido(thioperoxoic) *OS*-acid	(1O,1S,2N; OS; SH)
–$S(=NH)_2$-SeH	sulfonodiimidoselenoic acid	(1Se,2N)
–$S(=NH)_2$-TeH	sulfonodiimidotelluroic acid	(1Te,2N)
–S(O)(=NNH_2)-OH	sulfonohydrazonic acid	
–S(O)(=NNH_2)-OOH	sulfonohydrazonoperoxoic acid	(3O,1NN; OO)
–S(S)(=NNH_2)-OOH	sulfonohydrazonoperoxothioic acid	(2O,1S,1NN; OO)
–S(S)(=NNH_2)-OH	sulfonohydrazonothioic *O*-acid	(1O,1S,1NN; OH)
–S(O)(=NNH_2)-SH	sulfonohydrazonothioic *S*-acid	(1O,1S,1NN; SH)
–$S(=NNH_2)_2OH$	sulfonodihyrazonic acid	
–$S(=NNH_2)_2$-OOH	sulfonodihydrazonoperoxoic acid	(2O,2NN; OO)
–$S(=NNH_2)_2$-SOH	sulfonodihydrazono(thioperoxoic) *SO*-acid	(1O,1S,2NN; SO, OH)
–$S(=NNH_2)_2$-SH	sulfonodihydrazonothioic acid	(1S,2NN)

Table 4.4 Complete list of suffixes and functional replacement analogues (when present) for IUPAC preferred names, in decreasing order of seniority

1.	Carboxylic acids	–COOH	carboxylic acid
		–(C)OOH	oic acid
	Carboperoxoic acids	–CO-OOH	carboperoxoic acid
		–(C)O-OOH	peroxoic acid

	Carboperoxoic acids modified by replacement with S, Se, and/or Te		
		–CS-OOH	carboperoxothioic acid
		–(C)S-OOH	peroxothioic acid
		–CSe-OOH	carboperoxoselenoic acid
		–(C)Se-OOH	peroxoselenoic acid
		–CO-SOH	carbo(thioperoxoic) *SO*-acid
		–(C)O-SOH	(thioperoxoic) *SO*-acid
		–CO-OSH	carbo(thioperoxoic) *OS*-acid
		–(C)O-OSH	(thioperoxoic) *OS*-acid
	Carboxylic acids modified by replacement with S, Se, and/or Te		
		–CS-OH	carbothioic *O*-acid
		–(C)S-OH	thioic *O*-acid
		–CO-SH	carbothioic *S*-acid
		–(C)O-SH	thioic *S*-acid
		–CO-SeH	carboselenoic *Se*-acid
		–(C)O-SeH	selenoic *Se*-acid
		–CS-SH	carbodithioic acid
		–(C)S-SH	dithioic acid
2.	Carboximidic acids	–C(=NH)-OH	carboximidic acid
		–(C)(=NH)-OH	imidic acid
	Carboximidoperoxoic acids	–C(=NH)-OOH	carboximidoperoxoic acid
		–(C)(=NH)-OOH	imidoperoxoic acid
	Carboximidoperoxoic acids modified by replacement with S, Se, and/or Te		
		–C(=NH)-SOH	carboximido(thioperoxoic) *SO*-acid
		–(C)(=NH)-SOH	imido(thioperoxoic) *SO*-acid
		–C(=NH)-OSH	carboximido(thioperoxoic) *OS*-acid
		–(C)(=NH)-OSH	imido(thioperoxoic) *OS*-acid
		–C(=NH)-SSH	carbo(dithioperox)imidic acid
		–(C)(=NH)-SSH	(dithioperox)imidic acid
		–C(=NH)-SeSH	carboximido(selenothioperoxoic) *SeS*-acid
		–(C)(=NH)-SeSH	imido(selenothioperoxoic) *SeS*-acid
	Carboximidic acids modified by replacement with S, Se, and/or Te		
		–C(=NH)-SH	carboximidothioic acid
		–(C)(=NH)-SH	imidothioic acid
3.	Carbohydrazonic acids	–C(=NH$_2$)-OH	carbohydrazonic acid
		–(C)(=NNH$_2$)-OH	hydrazonic acid
	Carbohydrazonoperoxoic acids	–C(=NNH$_2$)-OOH	carbohydrazonoperoxoic acid
		–(C)(=NNH$_2$)-OOH	hydrazonoperoxoic acid
	Carbohydrazonoperoxoic acids modified by replacement with S, Se, and/or Te		
		–C(=NNH$_2$)-SOH	carbohydrazono(thioperoxoic) *SO*-acid
		–(C)(=NNH$_2$)-SOH	hydrazono(thioperoxoic) *SO*-acid
		–C(=NNH$_2$)-OSH	carbohydrazono(thioperoxoic) *OS*-acid
		–(C)(=NNH$_2$)-OSH	hydrazono(thioperoxoic) *OS*-acid

	–C(=NNH$_2$)-TeTeH	carbo(ditelluroperoxo)hydrazonic acid
	–(C)(=NNH$_2$)-TeTeH	(ditelluroperoxo)hydrazonic acid
Carbohydrazonic acids modified by replacement with S, Se, and/or Te		
	–C(=NNH$_2$)-SH	carbohydrazonothioic acid
	–(C)(=NNH$_2$)-SH	hydrazonothioic acid
4. Sulfonic acids	–SO$_2$-OH	sulfonic acid
Sulfonoperoxoic acids	–SO$_2$-OOH	sulfonoperoxoic acid
Sulfonoperoxoic acids modified by replacement with S, Se and/or Te		
	–S(O)(S)-OOH	sulfonoperoxothioic acid
	–SO$_2$-SOH	sulfono(thioperoxoic) *SO*-acid
	–SO$_2$-OSH	sulfono(thioperoxoic) *OS*-acid
	–SS$_2$-OOH	sulfonoperoxodithioic acid
Sulfonic acids modified by replacement with S, Se and/or Te		
	–SO$_2$-SH	sulfonothioic *S*-acid
	–S(O)(S)-OH	sulfonothioic *O*-acid
	–S(S)(S)-SH	sulfonotrithioic acid
5. Sulfonimidic acids	–S(O)(=NH)-OH	sulfonimidic acid
Sulfonimidoperoxoic acids	–S(O)(=NH)-OOH	sulfonimidoperoxoic acid
Sulfonimidoperoxoic acids modified by replacement with S, Se, or Te		
	–S(O)(=NH)-SOH	sulfonimido(thioperoxoic) *SO*-acid
	–S(O)(=NH)-OSH	sulfonimido(thioperoxoic) *OS*-acid
Sulfonimidic acids modified by replacement with S, Se or Te		
	–S(O)(=NH)-SH	sulfonimidothioic *S*-acid
6. Sulfonodiimidic acids	–S(=NH)$_2$-OH	sulfonodiimidic acid
Sulfonodiimidoperoxoic acids	–S(=NH)$_2$-OOH	sulfonodiimidoperoxoic acid
Sulfonodiimidoperoxoic acids modified by replacement with S, Se, and/or Te		
	–S(=NH)$_2$-SOH	sulfonodiimido(thioperoxoic) *SO*-acid
	–S(=NH)$_2$-OSH	sulfonodiimido(thioperoxoic) *OS*-acid
Sulfonodiimidic acids modified by replacement with S, Se, and/or Te		
	–S(=NH)$_2$-SeH	sulfonodiimidoselenoic acid
7. Sulfonohydrazonic acids	–S(O)(=NNH$_2$)-OH	sulfonohydrazonic acid
Sulfonohydrazonoperoxoic acids	–S(O)(=NNH$_2$)-OOH	sulfonohydrazonoperoxoic acid
Sulfonohydrazonoperoxoic acids modified by replacement with S, Se, and/or Te		
	–S(S)(=NNH$_2$)-OOH	sulfonohydrazonoperoxothioic acid
Sulfonohydrazonic acids modified by replacement with S, Se and/or Te		
	–S(S)(=NNH$_2$)-OH	sulfonohydrazonothioic *O*-acid
	–S(O)(=NNH$_2$)-SH	sulfonohydrazonothioic *S*-acid
8. Sulfonodihydrazonic acids	–S(=NNH$_2$)$_2$-OH	sulfonodihydrazonic acids
Sulfonodihydrazonoperoxoic acid	–S(=NNH$_2$)$_2$-OOH	sulfonodihydrazonoperoxoic acid
Sulfonodihydrazonoperoxoic acids modified by replacement with S, Se, and/or Te		
	–S(=NNH$_2$)$_2$-SOH	sulfonodihydrazono(thioperoxoic) *SO*-acid
Sulfonodihydrazonic acids modified by replacement with S, Se, and/or Te		

	$\mathrm{–S(=NNH_2)_2\text{-}SH}$	sulfonodihydrazonothioic acid
9. Sulfinic acids	–SO-OH	sulfinic acid
Sulfinoperoxoic acid	–SO-OOH	sulfinoperoxoic acid
Sulfinoperoxoic acid modified by replacement with S, Se, and/or Te		
	–S(S)-OOH	sulfinoperoxothioic acid
	–SO-SOH	sulfino(thioperoxoic) *SO*-acid
	–SO-OSH	sulfino(thioperoxoic) *OS*-acid
Sulfinic acids modified by replacement with S, Se, and/or Te		
	–SS-OH	sulfinothioic *O*-acid
	–SO-SeH	sulfinoselenoic *Se*-acid
10. Sulfinimidic acids	–S(=NH)-OH	sulfinimidic acid
Sulfinimidoperoxoic acids	–(=NH)-OOH	sulfinimidoperoxoic acid
Sulfinimidoperoxoic acids modified by replacement with S, Se and/or Te		
	–S(=NH)-OSH	sulfinimido(thioperoxoic) *OS*-acid
Sulfinimidic acids modified by replacement with S, Se, and/or Te		
	–S(=NH)-SH	sulfinimidothioic acid
11. Sulfinohydrazonic acids	$\mathrm{–S(=NNH_2)\text{-}OH}$	sulfinohydrazonic acid
Sulfinohydrazonoperoxoic acids	$\mathrm{–S(=NNH_2)\text{-}OOH}$	sulfinohydrazonoperoxoic acid
Sulfinohydrazonoperoxoic acids modified by replacement with S, Se and/or Te		
	$\mathrm{–S(=NNH_2)\text{-}SSeH}$	sulfinohydrazono(selenothioperoxoic) *SSe*-acid
Sulfinohydrazonic acids modified by replacement with S, Se, and/or Te		
	$\mathrm{–S(=NNH_2)\text{-}TeH}$	sulfinohydrazonotelluroic acid
12. Selenonic acids	$\mathrm{–SeO_2\text{-}OH}$	selenonic acid (as for sulfonic acids)
13. Seleninic acids	–SeO-OH	seleninic acid (as for sulfinic acids)
14. Telluronic acids	$\mathrm{–TeO_2\text{-}OH}$	telluronic acid (as for sulfonic acids)
15. Tellurinic acids	–TeO-OH	tellurinic acid (as for sulfinic acids)
16. Carboxamides	$\mathrm{–CO\text{-}NH_2}$	carboxamide
	$\mathrm{–(C)O\text{-}NH_2}$	amide
Carboxamides modified by replacement with S, Se, and/or Te		
	$\mathrm{–CS\text{-}NH_2}$	carbothioamide
	$\mathrm{–(C)S\text{-}NH_2}$	thioamide
17. Carboximidamides	$\mathrm{–C(=NH)\text{-}NH_2}$	carboximidamide
	$\mathrm{–(C)(=NH)\text{-}NH_2}$	imidamide
18. Carbohydrazonamides	$\mathrm{–C(=NNH_2)\text{-}NH_2}$	carbohydrazonamide
	$\mathrm{–(C)(=NNH_2)\text{-}NH_2}$	hydrazonamide
19. Sulfonamides	$\mathrm{–SO_2\text{-}NH_2}$	sulfonamide
Sulfonamides modified by replacement with S, Se, and/or Te		

	$–S(O)(S)\text{-}NH_2$	sulfonothioamide
	$–S(S)(Se)\text{-}NH_2$	sulfonoselenothioamide
20. Sulfonimidamides	$–S(O)(=NH)\text{-}NH_2$	sulfonimidamide
Sulfonimidamides modified by replacement with S, Se, and/or Te		
	$–S(S)(=NH)\text{-}NH_2$	sulfonimidothioamide
21. Sulfonodiimidamides	$–S(=NH)_2\text{-}NH_2$	sulfonodiimidamide
22. Sulfonohydrazonamides	$–S(O)(=NNH_2)\text{-}NH_2$	sulfonohydrazonamide
Sulfonohydrazonamides modified by replacement with S, Se, and/or Te		
	$–S(S)(=NNH_2)\text{-}NH_2$	sulfonohydrazonothioamide
23. Sulfonodihydrazonamides	$–S(=NNH_2)_2\text{-}NH_2$	sulfonodihydrazonamide
24. Sulfinamides	$–SO\text{-}NH_2$	sulfinamide
Sulfinamides modified by replacement with S, Se, and/or Te		
	$–S(Se)\text{-}NH_2$	sulfinoselenoamide
25. Sulfinimidamides	$–S(=NH)\text{-}NH_2$	sulfinimidamide
26. Sulfinohydrazonamides	$–S(=NNH_2)\text{-}NH_2$	sulfinohydrazonamide
27. Selenonamides	$–SeO_2\text{-}NH_2$	selenonamide (as for sulfonamides)
28. Seleninamides	$–SeO\text{-}NH_2$	seleninamide (as for sulfinamides)
29. Telluronamides	$–TeO_2\text{-}NH_2$	telluronamide (as for sulfonamides)
30. Tellurinamides	$–TeO\text{-}NH_2$	tellurinamide (as for sulfinamide)
31. Carbohydrazides	$–CO\text{-}NHNH_2$	carbohydrazide
	$–(C)O\text{-}NHNH_2$	hydrazide
Carbohydrazides modified by replacement with S, Se, and/or Te		
	$–CS\text{-}NHNH_2$	carbothiohydrazide
32. Carboximidohydrazides	$–C(=NH)\text{-}NHNH_2$	carboximidohydrazide
	$–(C)(=NH)\text{-}NHNH_2$	imidohydrazide
33. Carbohydrazonohydrazides	$–C(=NNH_2)\text{-}NHNH_2$	carbohydrazonohydrazide
	$–(C)(=NNH_2)\text{-}NHNH_2$	hydrazonohydrazide
34. Sulfonohydrazides	$–SO_2\text{-}NHNH_2$	sulfonohydrazide
Sulfonohydrazides modified by replacement with S, Se, and/or Te		
	$–S(O)(S)\text{-}NHNH_2$	sulfonothiohydrazide
35. Sulfonimidohydrazides	$–S(O)(=NH)\text{-}NHNH_2$	sulfonimidohydrazide
Sulfonimidohydrazides modified by replacement with S, Se, and/or Te		
	$–S(Se)(=NH)\text{-}NHNH_2$	sulfonimidoselenohydrazide
36. Sulfonodiimidohydrazides	$–S(=NH)_2\text{-}NHNH_2$	sulfonodiimidohydrazide
37. Sulfonohydrazonohydrazides	$–S(O)(=NNH_2)\text{-}NHNH_2$	sulfonohydrazonohydrazide
Sulfonohydrazonohydrazides modified by replacement with S, Se, andor Te		
	$–S(Te)(=NNH_2)\text{-}NHNH_2$	sulfonohydrazonotellurohydrazide
38. Sulfonodihydrazonohydrazides	$–S(=NNH_2)_2\text{-}NHNH_2$	sulfonodihydrazonohydrazide
39. Sulfinohydrazides	$–S(O)\text{-}NHNH_2$	sulfinohydrazide

Sulfinohydrazides modified by replacement with S, Se, and/or Te		
	$-S(Se)\text{-}NHNH_2$	sulfinoselenohydrazide
40. Sulfinimidohydrazides	$-S(=NH)\text{-}NHNH_2$	sulfinimidohydrazide
41. Sulfinohydrazonohydrazides	$-S(=NNH_2)\text{-}NHNH_2$	sulfinohydrazonohydrazide
42. Selenonohydrazides	$-SeO_2\text{-}NHNH_2$	selenonohydrazide (as for sulfonohydrazides)
43. Seleninohydrazides	$-Se(O)\text{-}NHNH_2$	seleninohydrazide (as for sulfinohydrazides)
44. Telluronohydrazides	$-TeO_2\text{-}NHNH_2$	telluronohydrazide (as for sulfonohydrazides)
45. Tellurinohydrazides	$-Te(O)\text{-}NHNH_2$	tellurinohydrazide (as for sulfinohydrazides)
46. Nitriles	–CN –(C)N	carbonitrile nitrile
47. Aldehydes	–CHO –(C)HO	carbaldehyde al
Aldehydes modified by replacement with S, Se, and/or Te		
	–CHS –(C)HS	carbothialdehyde thial
	–CHSe –(C)HSe	carboselenaldehyde selenal
	–CHTe –(C)HTe	carbotelluraldehyde tellural
48. Ketones, pseudoketones, and heterones	>(C)=O	one
Ketones, pseudoketones, and heterones modified by replacement with S, Se, and/or Te		
	>(C)=S >(C)=Se >(C)=Te	thione selone (not selenone) tellone (not tellurone)
49. Hydroxy compounds	–OH	ol
Hydroxy compounds modified by replacement with S, Se, and/or Te		
	–SH –SeH –TeH	thiol selenol tellurol
50. Hydroperoxides	–OOH	peroxol
Hydroperoxides modified by replacement with S, Se, and/or Te		
	–OSH –SOH	*OS*-thioperoxol *SO*-thioperoxol (not sulfenic acid)
51. Amines	$-NH_2$	amine
52. Imines	=NH	imine

P-44 SENIORITY ORDER FOR PARENT STRUCTURES

A parent structure is defined (P-15.1.1 and P-15.1.2) as a parent hydride, for example methane, a functionalized parent hydride, for example, cyclohexanol, or a functional parent compound, for example, acetic acid. For choice of the preferred IUPAC name based on a senior parent structure, see P-45.

P-44.0 Introduction
P-44.1 Seniority order for parent structures

P-44.2 Seniority order only for rings and ring systems
P-44.3 Seniority of acyclic chains (the principal chain)
P-44.4 Seniority criteria applicable to rings, ring systems, or acyclic chains

P-44.0 INTRODUCTION

The selection of a preferred parent structure is based on the seniority of classes (see P-41), which gives priority first to characteristic groups expressed as suffixes and then to parent hydrides when different classes are present. Section P-44.1 covers the selection of a preferred parent structure when different classes are involved and the selection between rings and chains in the same class. When there is a choice among cyclic parent hydrides, the senior ring or ring system is chosen in accord with the seniority order of rings and ring systems (see P-44.2). When there is a choice among acyclic parent hydrides a principal chain must be chosen (see P-44.3). The three seniority orders, for classes, rings and ring systems, and the principal chain, are expressed in a general seniority order called 'seniority order for parent structures'. Section P-44.4 covers criteria for selection of a senior parent structure applicable to either rings, ring systems, or acyclic chains.

A thorough revision and extension of the seniority order of classes, of rings and ring systems, and for selecting the principal chain was needed in the context of preferred names. This revision incorporates a major change from earlier recommendations given in the 1979 edition (ref. 1) and the 1993 Guide (ref. 2).

> In acyclic parent structures the order of seniority between unsaturation and length of chain given in earlier recommendations is reversed. Thus, the first criterion to be considered in choosing a preferred parent acyclic chain is the length of the chain; unsaturation is now the second criterion.

Note 1: Since the senior parent structure can occur in a compound in multiple ways, several plausible, unambiguous names can be generated. The criteria necessary to select a preferred IUPAC name are described in P-45; thus, traditional criteria related to substituent groups are not incorporated in this Section.

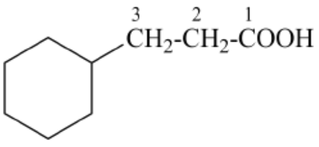
Note 2: Criteria related to nonstandard bonding have been incorporated into the criteria applicable to either rings, ring systems, or acyclic chains (P-44.4); hierarchically, they come after the criteria related to unsaturation (double bonds) and before those related to indicated hydrogen atoms.

P-44.1 SENIORITY ORDER FOR PARENT STRUCTURES

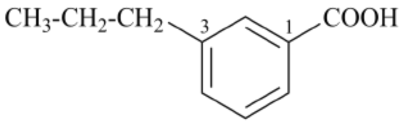
When there is a choice, the senior parent structure is chosen by applying the following criteria, in order, until a decision is reached. These criteria must always be applied before those applicable to rings and ring systems (see P-44.2) and to chains (see P-44.3). Then criteria applicable to both chains and rings or ring systems given in P-44.4 are considered.

P-44.1.1 The senior parent structure has the maximum number of substituents corresponding to the principal characteristic group (suffix) or senior parent hydride in accord with the seniority of classes (P-41) and the seniority of suffixes (P-43).

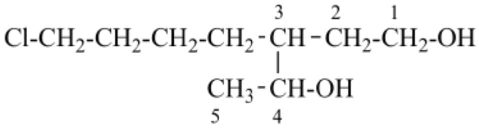
Examples:



3-cyclohexylpropanoic acid (PIN)
cyclohexanepropanoic acid (see P-15.6)



3-propylbenzoic acid (PIN)



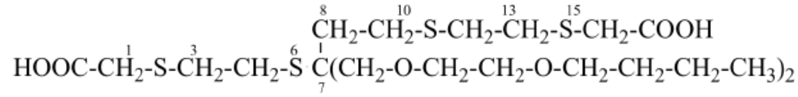
$$\text{Cl-CH}_2\text{-CH}_2\text{-CH}_2\text{-CH}_2\text{-}\underset{\substack{|\\ \text{CH}_3\text{-CH-OH}\\ 5\quad\ 4}}{\overset{3}{\text{CH}}}\text{-}\overset{2}{\text{CH}_2}\text{-}\overset{1}{\text{CH}_2}\text{-OH}$$

3-(4-chlorobutyl)pentane-1,4-diol (PIN)
[not 7-chloro-3-(1-hydroxyethyl)heptan-1-ol;
there are two of the principal characteristic groups in the parent of the PIN
and only one in the other name]
[not 3-(4-chlorobutyl)pentane-2,5-diol;
the locant set '1,4' for the principal characteristic groups of the PIN is lower than '2,5']

$NH_2\text{-}NH\text{-}COOH$
hydrazinecarboxylic acid (PIN)

$H_3Si\text{-}CH_2\text{-}CH_2\text{-}COOH$
3-silylpropanoic acid (PIN)

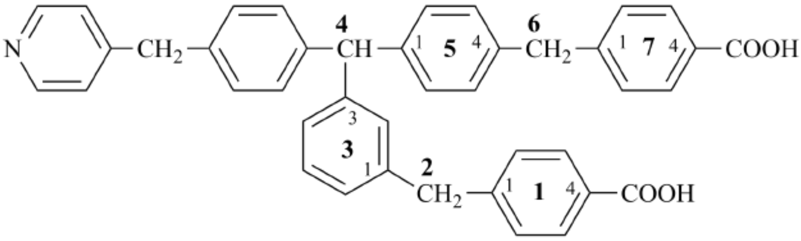
$HOOC\text{-}SiH_2\text{-}CH_2\text{-}CH_3$
ethylsilanecarboxylic acid (PIN)



$$\begin{array}{l} \qquad\qquad\qquad\qquad\qquad\quad \overset{8}{C}H_2\text{-}\overset{10}{C}H_2\text{-}S\text{-}CH_2\text{-}\overset{13}{C}H_2\text{-}\overset{15}{S}\text{-}CH_2\text{-}COOH \\ HOOC\text{-}\overset{1}{C}H_2\text{-}S\text{-}\overset{3}{C}H_2\text{-}CH_2\text{-}\overset{6}{S}\ \underset{7}{\overset{|}{C}}(CH_2\text{-}O\text{-}CH_2\text{-}CH_2\text{-}O\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}CH_3)_2 \end{array}$$

7,7-bis[(2-butoxyethoxy)methyl]-3,6,10,13-tetrathiapentadecane-1,15-dioic acid (PIN)
[not 9-[(2-butoxyethoxy)methyl]-9-({2-[(carboxymethyl)sulfanyl]ethyl}sulfanyl)-11,14-dioxa-3,6-dithiaoctadecan-1-oic acid;
nor 7-[(2-butoxyethoxy)methyl]-7-[2-({2-[(carboxymethyl)sulfanyl]ethyl}sulfanyl)ethyl]-9,12-dioxa-3,6-dithiahexadecan-1-oic acid;
there are two of the principal characteristic group in the parent of the PIN
and only one in the other names]

$H_3Si\text{-}CH_2\text{-}CH_2\text{-}SiH_2\text{-}CH_2\text{-}CH_2\text{-}SiH_3$
[silanediyldi(ethane-2,1-diyl)]bis(silane) (PIN)
(Si is senior to C, see P-44.1.2)
[not bis(2-silylethyl)silane;
the multiplicative preferred name expresses two occurrences of the parent hydride silane;
the substitutive name expresses only one]



4-{4-[(pyridin-4-yl)methyl]phenyl}-1,7(1),3(1,3),5(1,4)-tetrabenzenaheptaphane-1^4,7^4-dicarboxylic acid (PIN)
[not 4-{[4-(4-carboxyphenyl)methyl]phenyl}-1(4)-pyridina-3(1,4),5(1,3),7(1)-tribenzenaheptaphane-7^4-carboxylic acid;
nor 4-{[3-(4-carboxyphenyl)methyl]phenyl}-1(4)-pyridina-3,5(1,4),7(1)-tribenzenaheptaphane-7^4-carboxylic acid;
there are two of the principal characteristic group in the PIN and only one in the other names]

P-44.1.2 The senior parent structure, whether cyclic or acyclic, has the senior atom in accordance with the seniority of classes (see P-41) expressed by the following decreasing element order: N > P > As > Sb > Bi > Si > Ge > Sn > Pb > B > Al > Ga > In > Tl > O > S > Se > Te > C. This criterion is applied to select the senior atom in parents and to choose between rings and chains. It is not used to choose between rings or to select the principal chain modified by skeletal replacement (‘a’) nomenclature. If the most senior class is a ring system or a chain modified by skeletal replacement (‘a’) nomenclature, the senior parent is chosen among all rings (see P-44.2) or chains (see P-44.3) respectively.

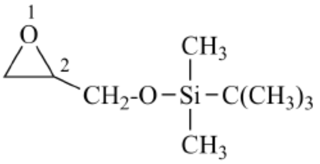
P-44.1.2.1 When two or more atoms denoting different classes are present in a compound, and when the choice for parent compound is between these atoms, the parent compound is the one belonging to the class cited first in the seniority of classes given above. A single senior atom is sufficient to give seniority to the parent hydride.

This rule is broader than Rule D-1.34 in the 1979 Recommendations (ref. 1) that referred to compounds where the heteroatoms were directly attached to each other.

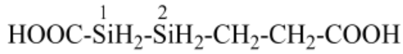
Examples:

$Si(CH_3)_4$
tetramethylsilane (PIN)
(Si is senior to C)

$CH_3\text{-}PH\text{-}SiH_3$
methyl(silyl)phosphane (PIN)
(P is senior to Si and C)

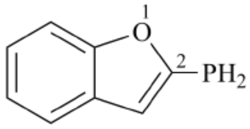


tert-butyldi(methyl)(oxiranylmethoxy)silane (PIN)
(Si is senior to O)

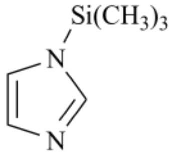


$\mathrm{HOOC\text{-}\overset{1}{Si}H_2\text{-}\overset{2}{Si}H_2\text{-}CH_2\text{-}CH_2\text{-}COOH}$

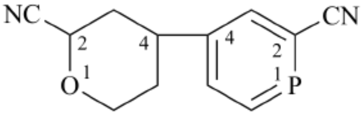
2-(2-carboxyethyl)disilane-1-carboxylic acid (PIN)
(Si is senior to C)



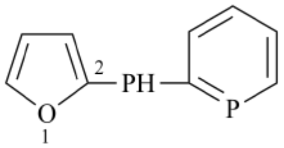
(1-benzofuran-2-yl)phosphane (PIN)
(P is senior to O)



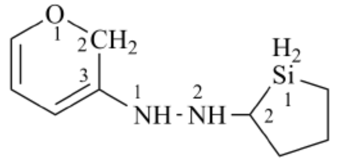
1-(trimethylsilyl)-1*H*-imidazole (PIN)
(N is senior to Si)



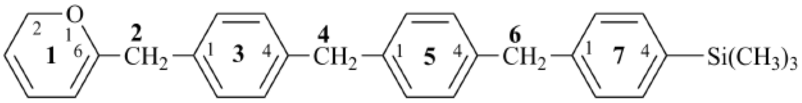
4-(2-cyanophosphinin-4-yl)oxane-2-carbonitrile (PIN)
(O > P; see P-44.2;
senior parent cannot be chosen by P-44.1.2)



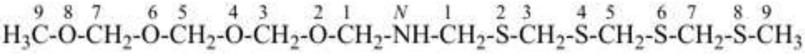
2-[(phosphinin-2-yl)phosphanyl]furan (PIN)
(P-ring is senior to P-chain; O-ring is senior to P-ring)



1-(2*H*-pyran-3-yl)-2-(silolan-2-yl)hydrazine (PIN)
(N > Si > O)

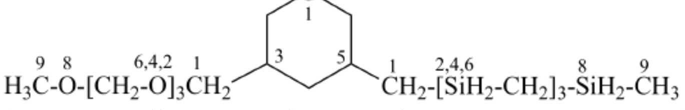


trimethyl[1^2H-1(6)-pyrana-3,5(1,4),7(1)-tribenzenaheptaphan-7^4-yl]silane (PIN)
(Si is senior to O)



$\mathrm{\overset{9}{H_3C}\text{-}\overset{8}{O}\text{-}\overset{7}{C}H_2\text{-}\overset{6}{O}\text{-}\overset{5}{C}H_2\text{-}\overset{4}{O}\text{-}\overset{3}{C}H_2\text{-}\overset{2}{O}\text{-}\overset{1}{C}H_2\text{-}\overset{\mathit{N}}{N}H\text{-}\overset{1}{C}H_2\text{-}\overset{2}{S}\text{-}\overset{3}{C}H_2\text{-}\overset{4}{S}\text{-}\overset{5}{C}H_2\text{-}\overset{6}{S}\text{-}\overset{7}{C}H_2\text{-}\overset{8}{S}\text{-}\overset{9}{C}H_3}$

N-(2,4,6,8-tetrathianonan-1-yl)-2,4,6,8-tetraoxanonan-1-amine (PIN)
[O > S; see P-44.3;
senior parent cannot be chosen by P-44.1.2]



1-[5-(2,4,6,8-tetrasilanonan-1-yl)oxan-3-yl]-2,4,6,8-tetraoxanonane (PIN)
[O-chain > Si-chain (see P-44.3;
senior parent cannot be chosen by P-44.1.2)]

P-44.1.2.2 Systems composed of rings and chains (exclusive of linear phanes)

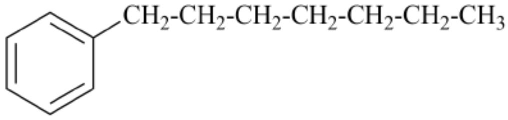
Two methods are recognized to name systems composed of rings and chains (exclusive of linear phanes).

(1) Within the same class, a ring or ring system has seniority over a chain. When a ring and a chain contain the same senior element, the ring is chosen as parent. Rings and chains are chosen regardless of their degree of hydrogenation. As a consequence, this approach prefers the choice of a ring over a chain in systems composed of cyclic and acyclic hydrocarbons.

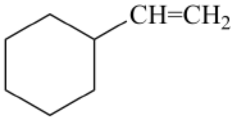
(2) The context may favor the ring or the chain, so that, for example, substituents may be treated alike or an unsaturated acyclic structure may be recognized, or the one chosen has the greater number of skeletal atoms in the ring or in the principal chain of the acyclic structure.

In the examples that follow, when a choice is possible, names formed by both methods are given. For selection of a preferred IUPAC name, see P-52.2.8.

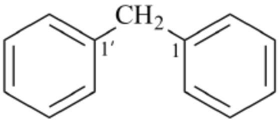
Examples:



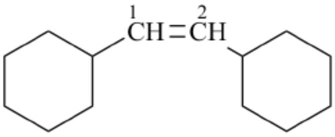
(1) heptylbenzene (PIN)
(ring is senior to chain)
(2) 1-phenylheptane
(chain has greater number of skeletal atoms)



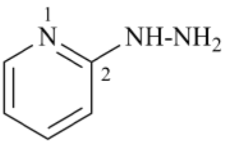
(1) ethenylcyclohexane (PIN)
(ring is senior to chain)
(2) cyclohexylethene
(emphasizes unsaturation)



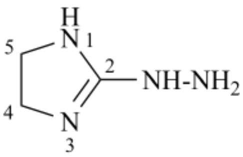
(1) 1,1′-methylenedibenzene (PIN)
(ring is senior to chain)
(2) diphenylmethane
(treats phenyl groups alike as substituents)



(1) 1,1′-(ethene-1,2-diyl)dicyclohexane (PIN)
(ring is senior to chain)
(2) 1,2-dicyclohexylethene
(emphasizes unsaturation)



(1) 2-hydrazinylpyridine (PIN)
(ring is senior to chain)
(2) (pyridin-2-yl)hydrazine
(pyridin-2-yl)diazane



(1) 2-hydrazinyl-4,5-dihydro-1*H*-imidazole (PIN)
2-diazanyl-4,5-dihydro-1*H*-imidazole
(ring is senior to chain)
(2) (4,5-dihydro-1*H*-imidazol-2-yl)hydrazine

P-44.1.3 Seniority order only for rings and ring systems. Criteria that apply only when the choice for parent structure is between two or more rings or ring systems are given in P-44.2.

P-44.1.4 Seniority among acyclic chains (the principal chain). Criteria that apply only when the choice for parent structure is between two or more acyclic chains are given in P-44.3.

P-44.1.5 Criteria applicable to rings, ring systems, or acyclic chains, such as unsaturation, the presence of skeletal atoms with different bonding numbers, isotopically modified compounds, and stereochemical configurations are given in P-44.4.

P-44.2 SENIORITY ORDER ONLY FOR RINGS AND RING SYSTEMS

P-44.2.1 Criteria general to all rings and ring systems (other than phanes, both cyclic and linear, for which see P-44.2.2.2.2 and P-44.2.2.2.6, respectively)
P-44.2.2 Criteria specific to a particular kind of ring or ring system

P-44.2.1 If application of P-44.1 does not effect a choice, general criteria for determining ring seniority given below are applied successively until there are no alternatives remaining. These criteria are listed first and then separately illustrated in P-44.2.1.2 through P-44.2.1.8, below.

The senior ring or ring system:

(a) is a heterocycle;

(b) has at least one nitrogen atom;

(c) has at least one heteroatom (in the absence of nitrogen) that occurs earlier in the following sequence: F > Cl > Br > I > O > S > Se > Te > P > As > Sb > Bi > Si > Ge > Sn > Pb > B > Al > Ga > In > Tl;

(d) has the greater number of rings;

(e) has the greater number of skeletal atoms;

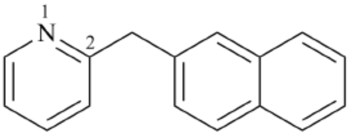
(f) has the greater number of heteroatoms of any kind;

(g) has the greater number of heteroatoms occurring earlier in the sequence: F > Cl > Br > I > O > S > Se > Te > N > P > As > Sb > Bi > Si > Ge > Sn > Pb > B > Al > Ga > In > Tl.

P-44.2.1.1 General methodology.

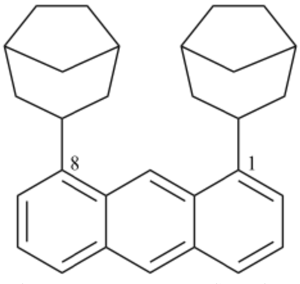
In order to apply P-44.2 after P-44.1 has failed to reach a conclusion, there must not be a characteristic group present in the compound, or the same number of a characteristic group must be present in all cyclic structures to be compared. In the following examples, as well as examples throughout P-44.2, seniority is expressed by the symbol '>' to be read as 'senior to'. In the case of larger structures the phrase 'is senior to' is cited between the senior structure and the less senior structure.

Examples (the symbol > means 'is senior to'):



2-[(naphthalen-2-yl)methyl]pyridine (PIN)
(pyridine > naphthalene)

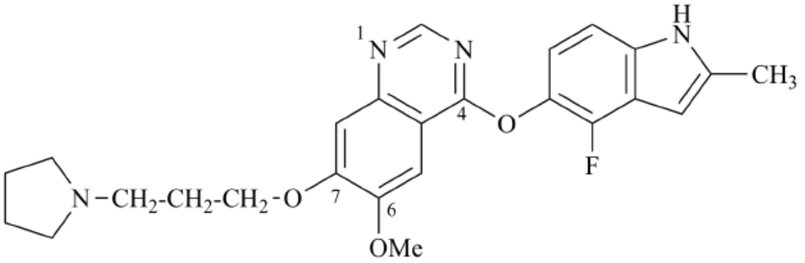
Note: In this compound, there is no characteristic group to be cited as suffix. One ring must be chosen as the senior ring that will serve as the parent hydride; the other ring will be cited as a prefix to the parent hydride. Criteria in P-44.2.1 must be applied starting from (a), in the order given, until a decision is reached. In this case, application of the first criterion (a) leads to a decision: the ring containing a nitrogen atom is selected as parent hydride; the naphthalene ring system is cited as a substituent.



1,8-di(bicyclo[3.2.1]octan-3-yl)anthracene (PIN)

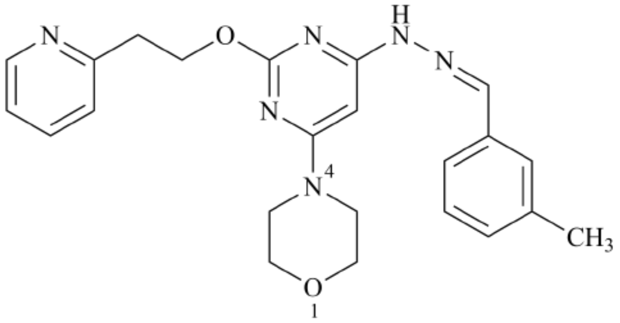
Note: In the above compound, there is no characteristic group to be cited as suffix. One ring must be chosen as the senior ring that will serve as the parent hydride; the other ring will be cited as a prefix to the parent hydride. Criteria in

P-44.2.1 must be applied starting from criterion (a), in the order given, until a decision is reached. In this case, application of criterion (d) leads to a decision: anthracene has more rings and is the parent structure; the bicyclo ring is cited as a substituent.



4-[(4-fluoro-2-methyl-1*H*-indol-5-yl)oxy]-6-methoxy-7-[3-(pyrrolidin-1-yl)propoxy]quinazoline (PIN)
(quinazoline > indole > pyrrolidine)

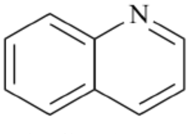
Note: In this compound, there are two ring systems and one ring. No characteristic group to be cited as suffix is present. Characteristic groups to be cited as prefixes are ignored at this stage of the selection of the senior ring or ring system. The ring system 'quinazoline' is selected as parent hydride after applying criteria (a), (b), and (d) in P-44.2.1; and finally it is criterion (e) that permits a decision to be reached between 'quinazoline' and 'indole'. Quinazoline is the parent hydride and both indole and pyrrolidine are included in the substituents cited as prefixes.



4-(6-{2-[(3-methylphenyl)methylidene]hydrazin-1-yl}-2-[2-(pyridin-2-yl)ethoxy]pyrimidin-4-yl)morpholine (PIN)
(morpholine > pyrimidine > pyridine > benzene)

Note: In this compound, 'morpholine' is chosen as parent hydride, as a decision in the selection of the senior ring cannot be made until criterion (g) in P-44.2.1 is reached. The rings benzene, pyridine, and pyrimidine are expressed within the substituent prefixes.

P-44.2.1.2 The senior ring or ring system is a heterocycle [criterion (a) in P-44.2.1]. Example (the symbol > means 'is senior to'):



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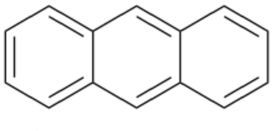
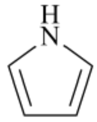


quinoline (PIN)

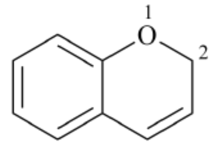
anthracene (PIN)

P-44.2.1.3 The senior ring or ring system has at least one nitrogen ring atom [criterion (b) in P-44.2.1]

Examples (the symbol > means 'is senior to'):

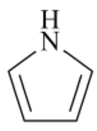


>



1*H*-pyrrole (PIN)

2*H*-1-benzopyran (PIN)
2*H*-chromene



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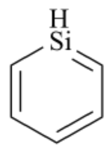
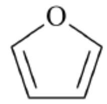


1*H*-pyrrole (PIN)

2*H*-siline (PIN)

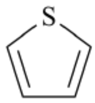
P-44.2.1.4 The senior ring or ring system has at least one heteroatom (in the absence of nitrogen) that occurs earlier in the following sequence: F > Cl > Br > I > O > S > Se > Te > P > As > Sb > Bi > Si > Ge > Sn > Pb > B > Al > Ga > In > Tl [criterion (c) in P-44.2.1].

Examples (the symbol > means ‘is senior to’):



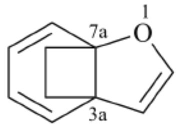
furan (PIN)

>



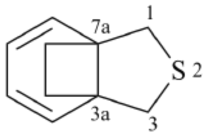
thiophene (PIN)

[O > S]



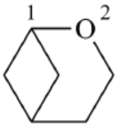
3a,7a-ethano-1-benzofuran (PIN)

>



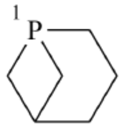
1*H*,3*H*-3a,7a-ethano-2-benzothiophene (PIN)

[O > S]



2-oxabicyclo[3.1.1]heptane (PIN)

>

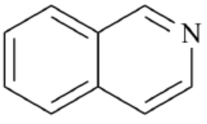


1-phosphabicyclo[3.1.1]heptane (PIN)

[O > P]

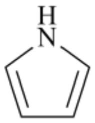
P-44.2.1.5 The senior ring or ring system has the greater number of rings [criterion (d) in P-44.2.1].

Example (the symbol > means ‘is senior to’):



isoquinoline (PIN)

>

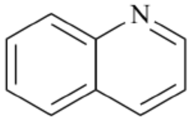


1*H*-pyrrole (PIN)

[2 rings > 1 ring]

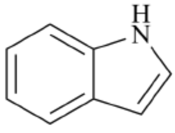
P-44.2.1.6 The senior ring or ring system has the greater number of skeletal atoms [criterion (e) in P-44.2.1].

Examples (the symbol > means ‘is senior to’):



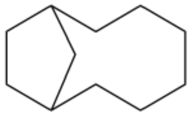
quinoline (PIN)

>



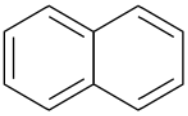
1*H*-indole (PIN)

[10 skeletal atoms > 9 skeletal atoms]



bicyclo[6.2.1]undecane (PIN)

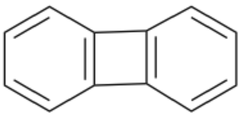
>



naphthalene (PIN)

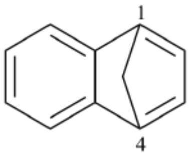
[11 skeletal atoms > 10 skeletal atoms]

Note: Because of the hierarchical nature of these criteria, this criterion regarding the number of skeletal atoms supersedes P-44.2.2.2, which prefers a fused ring to a bridged fused ring.



biphenylene (PIN)

>



1,4-methanonaphthalene (PIN)

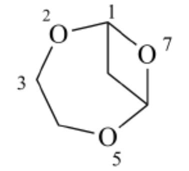
[12 skeletal atoms > 11 skeletal atoms]

Note: Because of the hierarchical nature of these criteria, this criterion regarding the number of skeletal atoms supersedes P-44.2.2.2, which prefers a fused ring to a bridged fused ring.

P-44.2.1.7 The senior ring or ring system has the greater number of heteroatoms of any kind [(criterion (f) in P-44.2.1]

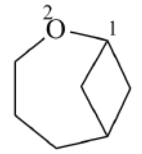
Examples (the symbol > means ‘is senior to’):

(1)



2,5,7-trioxabicyclo[4.1.1]octane (PIN)

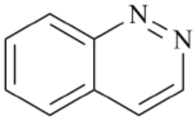
>



2-oxabicyclo[4.1.1]octane (PIN}

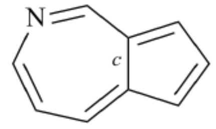
[3 heteroatoms > 1 heteroatom]

(2)



cinnoline (PIN)

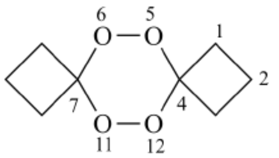
>



cyclopenta[*c*]azepine (PIN)

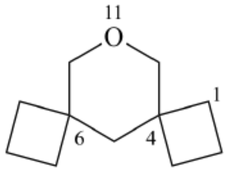
[2 heteroatoms > 1 heteroatom]

(3)



5,6,11,12-tetraoxadispiro[3.2.3^{7}.2^{4}]dodecane (PIN)

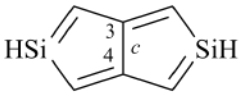
>



11-oxadispiro[3.1.3^{6}.3^{4}]dodecane (PIN)

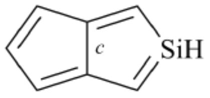
[4 heteroatoms > 1 heteroatom]

(4)



silolo[3,4-*c*]silole (PIN)

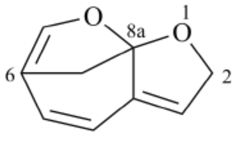
>



cyclopenta[*c*]silole (PIN)

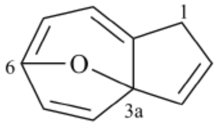
[2 heteroatoms > 1 heteroatom]

(5)



2*H*-6,8a-methanofuro[2,3-*b*]oxepine (PIN)

>



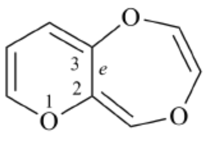
1*H*-3a,6-epoxyazulene (PIN)

[2 heteroatoms > 1 heteroatom]

P-44.2.1.8 The senior ring or ring system has the greater number of heteroatoms that occur earlier in the following sequence: F > Cl > Br > I > O > S > Se > Te > N > P > As > Sb > Bi > Si > Ge > Sn > Pb > B > Al > Ga > In > Tl [criterion (g) in P-44.2.1].

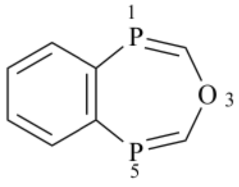
Examples (the symbol > means ‘is senior to’):

(1)



pyrano[3,2-*e*][1,4]dioxepine (PIN)

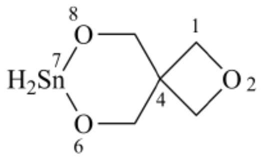
>



3,1,5-benzoxadiphosphepine (PIN)

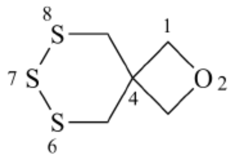
[3 heteroatoms = 3 heteroatoms; 3 oxygen atoms > 1 oxygen atom]

(2)



2,6,8-trioxa-7-stannaspiro[3.5]nonane (PIN)

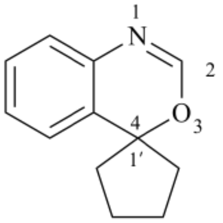
>



2-oxa-6,7,8-trithiaspiro[3.5]nonane (PIN)

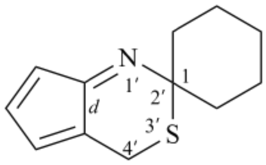
[4 heteroatoms = 4 heteroatoms; 3 oxygen atom > 1 oxygen atom]

(3)



spiro[[3,1]benzoxazine-4,1′-cyclopentane] (PIN)

>



4′*H*-spiro[cyclohexane-1,2′-cyclopenta[*d*][1,3]thiazine] (PIN)

[2 heteroatoms = 2 heteroatoms]
[1 nitrogen atom, 1 oxygen atom > 1 nitrogen atom, 1 sulfur atom]

P-44.2.2 Seniority criteria for determining ring seniority applicable to particular types of ring systems.

P-44.2.2.1 Monocycles (see P-22)

If P-44.2.1 does not provide a decision, further criteria applicable to monocyclic rings are found in P-44.4.

P-44.2.2.2 Polycyclic systems. The senior polycyclic ring system occurs first in the following list of polycyclic ring system types:

The seniority order between parent hydrides having the same number of identical heteroatoms, the same number of rings, and the same number of skeletal atoms is a change from previous practice. Seniority of polycyclic ring systems is now facilitated by a hierarchical order of ring systems, which includes cyclic and acyclic phane systems and ranks all ring systems in the order given in this recommendation.

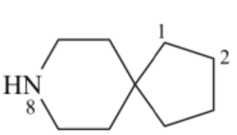
(a) spiro ring system (see P-24);
(b) cyclic phane system (see P-26);
(c) fused ring system (see P-25);
(d) bridged fused ring system (see P-25);
(e) nonfused bridged ring system (see P-23);
(f) linear phane system (see P-26);
(g) ring assembly (see P-28).

Choices within each type are illustrated in P-44.2.2.2.1 through P-44.2.2.2.7.

Further criteria applicable to polycyclic ring systems are found in P-44.4.

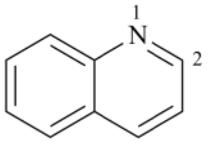
Examples (the symbol > means 'is senior to'):

(1)



8-azaspiro[4.5]decane (PIN)

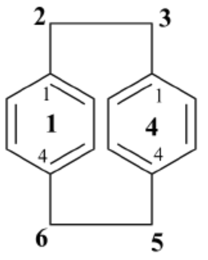
>



quinoline (PIN)

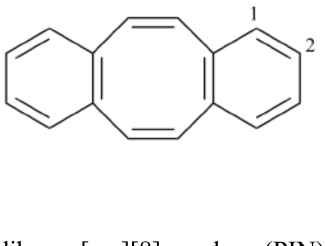
[spiro ring system (a) > fused ring system (c)]

(2)



1,4(1,4)-dibenzenacyclohexaphane (PIN)

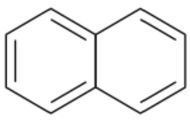
>



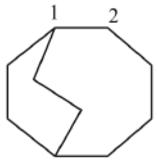
dibenzo[*a*,*e*][8]annulene (PIN)

[cyclic phane ring system (b) > fused ring system (c)]

(3)



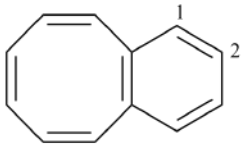
>



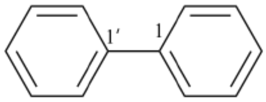
naphthalene (PIN) bicyclo[4.2.2]decane (PIN)

[fused ring system (c) > nonfused bridged ring system (e)]

(4)



>



benzo[8]annulene (PIN) 1,1′-biphenyl (PIN)

[fused ring system (c) > ring assembly (g)]

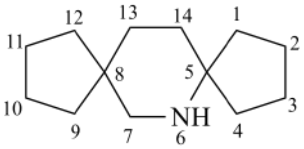
P-44.2.2.2.1 Seniority criteria for spiro ring systems given below are applied successively until no alternatives remain. These criteria are illustrated in P-44.2.2.2.1.1 through P-44.2.2.2.1.3. The senior spiro system:

(a) has the greater number of spiro fusions;
(b) consists of saturated monocyclic rings;
(c) consists of only discrete components.

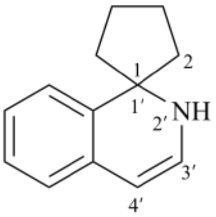
Further criteria applicable to spiro ring systems are found in P-44.4.

P-44.2.2.2.1.1 The senior spiro system has the greater number of spiro fusions [criterion (a) in P-44.2.2.2.1].

Example (the symbol > means 'is senior to'):



>

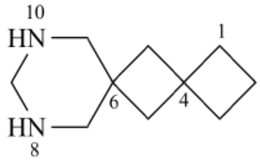


6-azadispiro[$4.2.4^{8}.2^{5}$]tetradecane (PIN) 2′*H*-spiro[cyclopentane-1,1′-isoquinoline] (PIN)

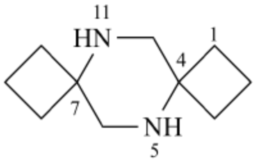
[2 spiro fusions > 1 spiro fusion]

P-44.2.2.2.1.2 The senior spiro system consists of only saturated monocyclic rings [criterion (b) in P-44.2.2.2.1] and has the lower locant(s) for spiro atom(s);

Example (the symbol > means 'is senior to'):



>



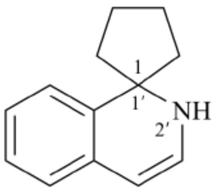
8,10-diazadispiro[$3.1.5^{6}.1^{4}$]dodecane (PIN) 5,11-diazadispiro[$3.2.3^{7}.2^{4}$]dodecane (PIN)

[saturated monocyclic rings each with 2 spiro fusions;
the locant set for spiro fusions '4,6' is lower that '4,7']

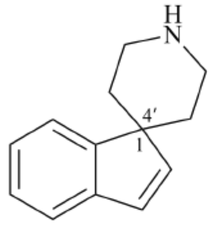
P-44.2.2.2.1.3 The senior spiro system consists only of discrete components [criterion (c) in P-44.2.2.2.1] and:

(a) has the senior component determined by criteria above and below for the appropriate type of ring or ring system when the components are compared in their order of seniority;

Example (the symbol > means ‘is senior to’):



>



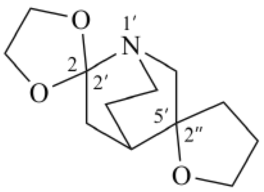
2′*H*-spiro[cyclopentane-1,1′-isoquinoline] (PIN)

spiro[indene-1,4′-piperidine] (PIN)

[isoquinoline > piperidine]

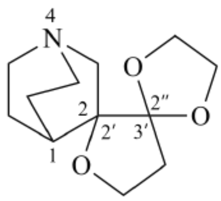
(b) has the senior component determined by criteria above and below for the appropriate kind of ring or ring system when compared in their order of citation in the name;

Example (the symbol > means ‘is senior to’):



(I)

>

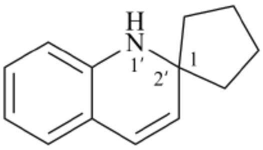


(II)

(**I**) 1′-azadispiro[[1,3]dioxolane-2,2′-bicyclo[2.2.2]octane-5′,2″-oxolane] (PIN)
is senior to
(**II**) 4-azadispiro[bicyclo[2.2.2]octane-2,2′-oxolane-3′,2″-[1,3]dioxolane] (PIN)
[first cited component dioxolane > bicyclo[2.2.2]octane]

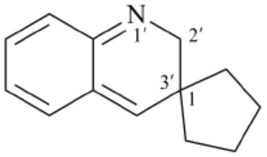
(c) has the lower locant(s) for the spiro atoms in the order of citation in the name.

Example (the symbol > means ‘is senior to’):



(I)

>



(II)

(**I**) 1′*H*-spiro[cyclopentane-1,2′-quinoline] (PIN)
is senior to
(**II**) 2′*H*-spiro[cyclopentane-1,3′-quinoline] (PIN)
[spiro fusion locant set 1,2′ in (**I**) is lower than 1,3′ in (**II**)]

P-44.2.2.2.2 Seniority criteria for the cyclic phane systems given below are applied successively until no alternatives remain. These criteria are illustrated in P-44.2.2.2.2.1 through P-44.2.2.2.2.8.

The senior cyclic phane system:

(a) is the one occurring earlier in the following list of basic phane skeletal ring systems: spiro, von Baeyer, monocyclic;

(b) has the senior amplificant, as defined by P-44.2.1.2 through P-44.2.1.8;

(c) has the lower superatom locant(s) for all amplificants, first as a set compared term by term order of increasing value and then in order of citation in the name;

(d) has the lower locant(s) for senior amplificants;

(e) has the lower set of attachment locants considered as a set when compared term by term in order of increasing numerical value;

(f) has the lower set of attachment locants when compared term by term in their order of citation in the name;

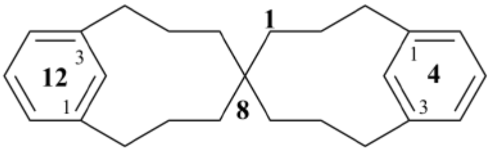
(g) has the lower locant(s) for heteroatoms introduced by skeletal replacement (‘a’) nomenclature without regard to kind;

(h) has the lower locant(s) for heteroatoms introduced by skeletal replacement (‘a’) nomenclature first cited in the following order: F > Cl > Br > I > O > S > Se > Te > N > P > As > Sb > Bi > Si > Ge > Sn > Pb > B > Al > Ga > In > Tl.

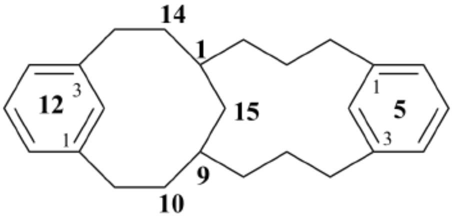
Further criteria applicable to cyclic phane systems are found in P-44.4.

P-44.2.2.2.2.1 The senior cyclic phane system occurs earlier in the following list of basic phane skeletal ring systems: spiro > nonfused bridged (von Baeyer) > monocyclic.

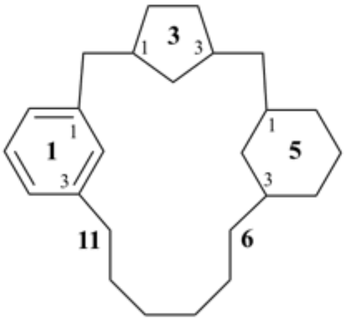
Examples (in order of decreasing seniority according to the criteria (a) in P-44.2.2.2.2):



4,12(1,3)-dibenzenaspiro[7.7]pentadecaphane (PIN)
(a spiro phane skeletal system)
is senior to



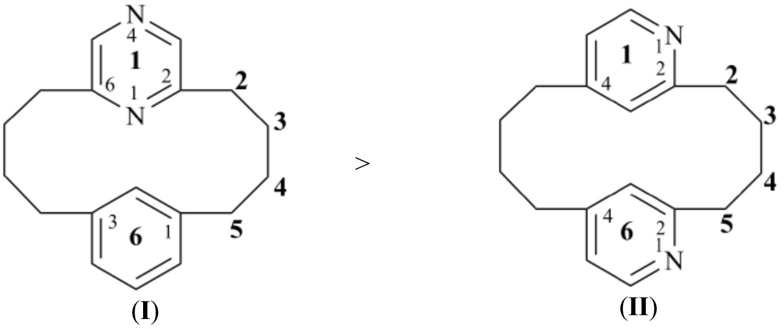
5,12(1,3)-dibenzenabicyclo[7.5.1]pentadecaphane (PIN)
(a von Baeyer phane skeletal system)
is senior to



1(1,3)-benzena-5(1,3)-cyclohexana-3(1,3)-cyclopentanacycloundecaphane (PIN)
(a monocyclic phane skeletal system)

P-44.2.2.2.2.2 The senior cyclic phane system has the senior amplificant, as defined by P-44.2.1.2 through P-44.2.1.8 [criterion (b) in P-44.2.2.2.2].

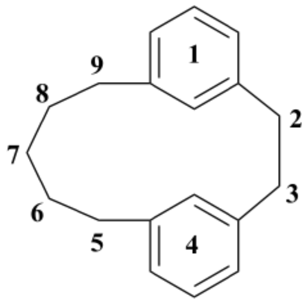
Example (the symbol > means 'is senior to'):



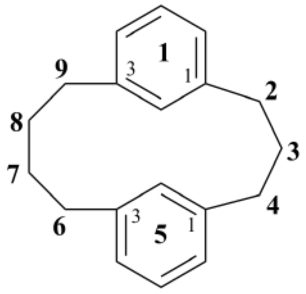
(**I**) 1(2,6)-pyrazina-6(1,3)-benzenacyclodecaphane (PIN)
is senior to
(**II**) 1,6(2,4)-dipyridinacyclodecaphane (PIN)
[pyrazine > pyridine]

P-44.2.2.2.2.3 The senior cyclic phane system has the lower superatom locant(s) for all amplificants, first as a set compared term by term in order of increasing numerical value and then in order of their citation in the name [criterion (c) in P-44.2.2.2.2].

Example (the symbol > means 'is senior to'):



>



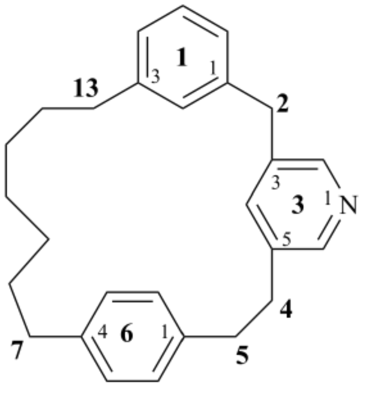
(**I**)
1,4(1,3)-dibenzenacyclononaphane (PIN)

(**II**)
1,5(1,3)-dibenzenacyclononaphane (PIN)

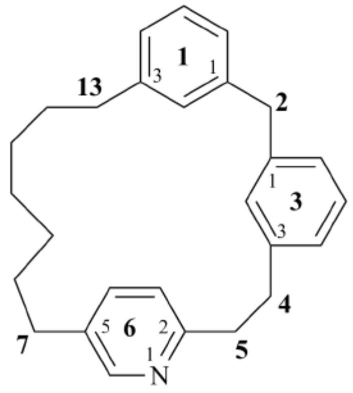
[superatom locant set '1,4' in (**I**) is lower than '1,5' in (**II**)]

P-44.2.2.2.2.4 The senior cyclic phane system has the lower locants for senior amplificants [criterion (d) in P-44.2.2.2.2].

Example (the symbol > means 'is senior to'):



>



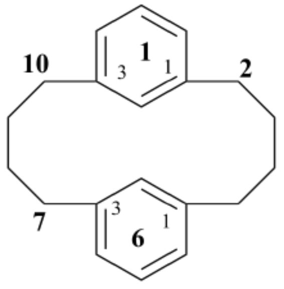
(**I**)

(**II**)

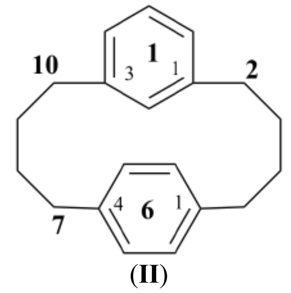
(**I**) 3(3,5)-pyridina-1(1,3),6(1,4)-dibenzenacyclotridecaphane (PIN)
is senior to
(**II**) 6(2,5)-pyridina-1,3(1,3)-dibenzenacyclotridecaphane (PIN)
[superatom locant '3' for the senior amplificant pyridine is lower than '6']

P-44.2.2.2.2.5 The senior cyclic phane system has the lower set of attachment locants considered as a set when compared term by term in order of increasing numerical value [criterion (e) in P-44.2.2.2.2].

Example (the symbol > means 'is senior to'):



>



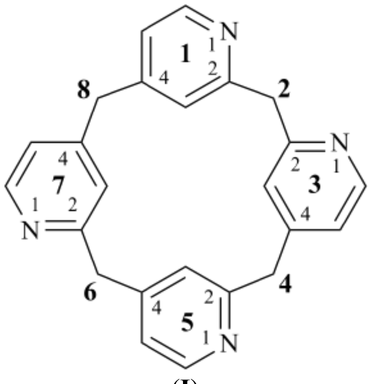
(**I**)
1,6(1,3)-dibenzenacyclodecaphane (PIN)

(**II**)
1(1,3),6(1,4)-dibenzenacyclodecaphane (PIN)

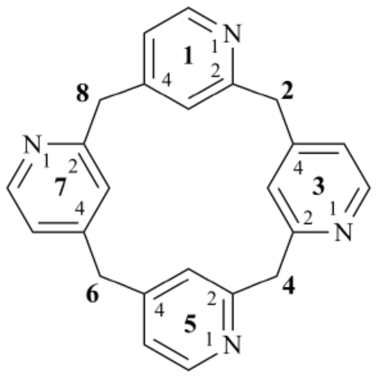
[the attachment locant set '(1,3)(1,3)' is lower than '(1,3)(1,4)']

P-44.2.2.2.2.6 The senior cyclic phane system has the lower set of attachment locants when compared term by term in their order of citation in the name [criterion (f) in P-44.2.2.2.2].

Example (the symbol > means ‘is senior to’):


1
N
1
2
4
2
8
7
4
1
2
N
3
N
1
2
4
6
4
5
4
2
1
N

>


1
N
1
2
4
2
8
N
1
2
7
4
3
4
1
2
N
6
4
5
4
2
1
N

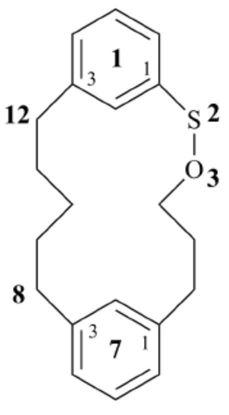
(I)

(II)

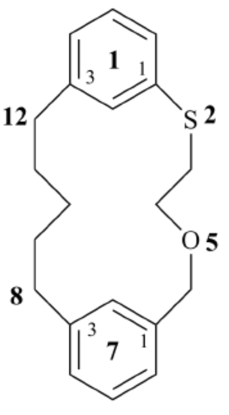
(I) 1,3,5,7(2,4)-tetrapyridinacyclooctaphane (PIN)
is senior to
(II) 1,5(2,4),3,7(4,2)-tetrapyridinacyclooctaphane (PIN)
[the attachment locant set ‘(2,4)(2,4)(2,4)(2,4)’ is lower than ‘(2,4)(2,4)(4,2)(4,2)’]

P-44.2.2.2.2.7 The senior cyclic phane system has the lower locant(s) for heteroatoms specified by skeletal replacement (‘a’) prefixes without regard to kind [criterion (g) in P-44.2.2.2.2].

Example (the symbol > means ‘is senior to’):


1
3
1
12
S 2
O 3
8
3
7
1

>

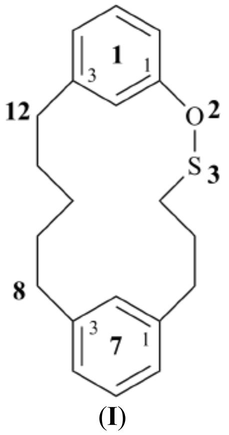

1
3
1
12
S 2
O 5
8
3
7
1

(I)

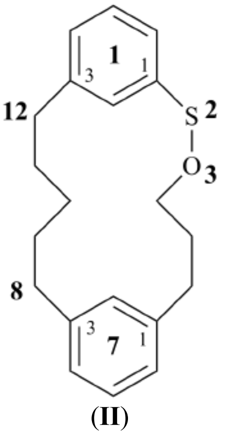
(II)

(I) 3-oxa-2-thia-1,7(1,3)-dibenzenacyclododecaphane (PIN)
is senior to
(II) 5-oxa-2-thia-1,7(1,3)-dibenzenacyclododecaphane (PIN)
[the heteroatom locant set ‘2,3’ is lower than ‘2,5’]

P-44.2.2.2.2.8 The senior cyclic phane system has the lower locant(s) for heteroatoms specified by skeletal replacement (‘a’) prefixes first cited in the following order: F > Cl > Br > I > O > S > Se > Te > N > P > As > Sb > Bi > Si > Ge > Sn > Pb > B > Al > Ga > In > Tl [criterion (h) in P-44.2.2.2.2]. Example (the symbol > means ‘is senior to’):


1
3
1
12
O 2
S 3
8
3
7
1

>


1
3
1
12
S 2
O 3
8
3
7
1

(I)

(II)

(I) 2-oxa-3-thia-1,7(1,3)-dibenzenacyclododecaphane (PIN)
is senior to
(II) 3-oxa-2-thia-1,7(1,3)-dibenzenacyclododecaphane (PIN)
[the locant ‘2’ for the senior heteroatom ‘O’ is lower than ‘3’]

P-44.2.2.2.3 Seniority criteria for fused ring systems given below are applied successively until no alternatives remain. The criteria are illustrated in P-44.2.2.2.3.1 through P-44.2.2.2.3.5. The senior fused ring system:

(a) has the larger individual ring component at first point of difference when their ring sizes are compared in order of decreasing size;

(b) has the greater number of rings in a horizontal row;

(c) has the lower letter(s) in the fusion descriptor when compared as a set; letters omitted in names are considered in the application of this criterion;

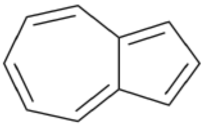
(d) has the lower number(s) in the fusion descriptor, in the order of appearance in the name; locants omitted in names are considered in application of this criterion;

(e) has the senior ring system component according to P-25.8 when its components are compared in order of decreasing seniority.

Further criteria applicable to fused ring systems are found in P-44.4.

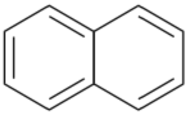
P-44.2.2.2.3.1 The senior fused ring system has the larger individual ring component at first point of difference when their ring sizes are compared in order of decreasing size [criterion (a) in P-44.2.2.2.3].

Example (the symbol > means 'is senior to'):



azulene (PIN)

>



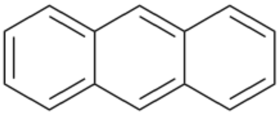
naphthalene (PIN)

[the ring size '7' in the ring set '7,5' is larger than '6' in the ring set '6,6']

P-44.2.2.2.3.2 The senior fused ring system has the greater number of rings in a horizontal row [criterion (b) in P-44.2.2.2.3].

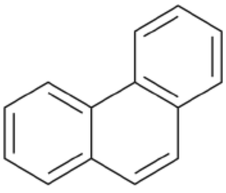
Example (the symbol > means 'is senior to'):

(1)



anthracene (PIN)

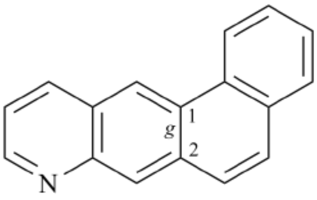
>



phenanthrene (PIN)

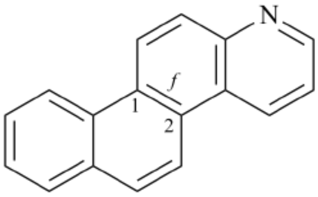
[three rings in the horizontal row is greater than two]

(2)



naphtho[1,2-*g*]quinoline (PIN)

>

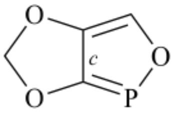


naphtho[2,1-*f*]quinoline (PIN)

[three rings in the horizontal row is greater than two]

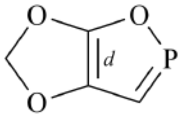
P-44.2.2.2.3.3 The senior fused ring system has the lower letter(s) alphabetically in the fusion descriptor when compared as a set; letters omitted in names are considered in the application of this criterion [criterion (c) in P-44.2.2.2.3].

Example (the symbol > means 'is senior to'):



5*H*-[1,3]dioxolo[4,5-*c*][1,2]oxaphosphole (PIN)

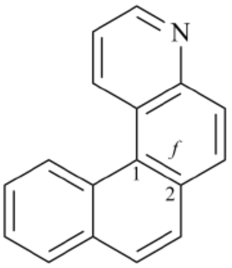
>



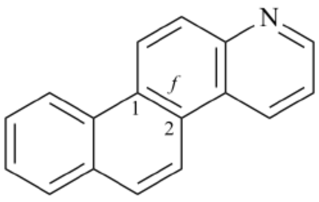
5*H*-[1,3]dioxolo[4,5-*d*][1,2]oxaphosphole (PIN)

[the letter 'c' in the fusion descriptor is lower alphabetically than 'd']

P-44.2.2.2.3.4 The senior fused ring system has the lower set of numbers in the fusion descriptor, in the order of appearance in a name; locants omitted in names are taken into consideration in application of this criterion [criterion (d) in P-44.2.2.2.3]. Example (the symbol > means 'is senior to'):



>



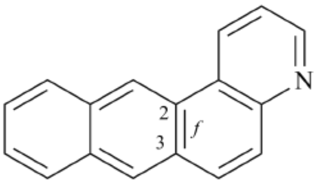
naphtho[1,2-*f*]quinoline (PIN)

naphtho[2,1-*f*]quinoline (PIN)

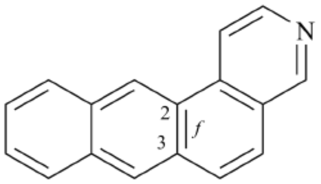
[the locant set ‘1,2’ in the fusion descriptor is lower than ‘2,1’]

P-44.2.2.2.3.5 The senior fused ring system has the senior ring system component according to P-25.8 when its components are compared in order of decreasing seniority [criterion (e) in P-44.2.2.2.3].

Example (the symbol > means ‘is senior to’):



>



naphtho[2,3-*f*]quinoline (PIN)

naphtho[2,3-*f*]isoquinoline (PIN)

[the senior ring system quinoline is senior to isoquinoline (see P-25.2.1, Table 2.8)]

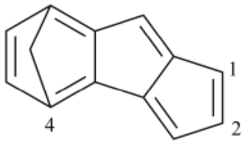
P-44.2.2.2.4 Seniority criteria for bridged fused ring systems given below are applied successively until no alternatives remain. The criteria are illustrated in P-44.2.2.2.4.1 through P-44.2.2.2.4.14. The senior bridged fused ring system:

(a) has the bridged ring system with the greater number of rings before bridging;
(b) is the bridged ring system with the greater number of ring atoms before bridging;
(c) is the bridged ring system with the fewer heteroatoms in the fused ring system before bridging;
(d) is the bridged ring system with the senior fused ring system before bridging according to P-44-2.2.2.3;
(e) has the lower set of locants for bridge attachments;
(f) has the lower locant(s) for heteroatoms in bridges, without regard to kind;
(g) has the lower locant(s) for heteroatoms in bridges, in the order: F > Cl > Br > I > O > S > Se > Te > N > P > As > Sb > Bi > Si > Ge > Sn > Pb > B > Al > Ga > In > Tl;
(h) has the fewer composite bridges;
(i) has the fewer dependent bridges;
(j) has fewer atoms in dependent bridges;
(k) has the greater number of divalent bridges;
(l) has the lower set of locants for attachment of independent bridges;
(m) has the lower set of locants for attachment of dependent bridges;
(n) has the fused ring system with the greater number of noncumulative double bonds before bridging.

Further criteria applicable to bridged fused ring systems are found in P-44.4.

P-44.2.2.2.4.1 The senior bridged fused ring system has the bridged ring system with the greater number of rings before bridging [criterion (a) in P-44.2.2.2.4].

Example (the symbol > means ‘is senior to’):



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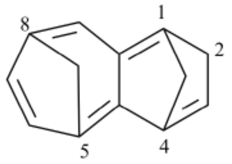


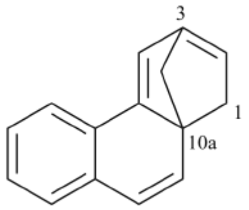
4,7-methanocyclopenta[*a*]indene (PIN)

2*H*-1,4:5,8-dimethanobenzo[7]annulene (PIN)

[three rings in the ring system before bridging is greater than two]

P-44.2.2.2.4.2 The senior bridged fused ring system is the bridged ring system with the greater number of ring atoms before bridging [criterion (b) in P-44.2.2.2.4].

Example (the symbol > means ‘is senior to’):



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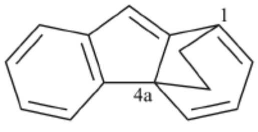
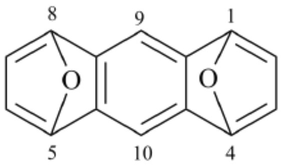


[fourteen ring atoms in the ring system before bridging is greater than thirteen]

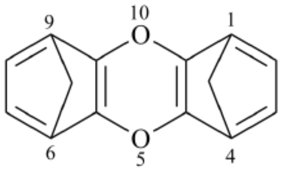
P-44.2.2.2.4.3 The senior bridged fused ring system is the bridged ring system with the fewer heteroatoms in the fused ring system before bridging [criterion (c) in P-44.2.2.2.4].

Example (the symbol > means 'is senior to'):



1,4:5,8-diepoxyanthracene (PIN)

>

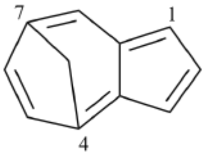


1,4:6,9-dimethanooxanthrene (PIN)

[zero heteroatoms in the fused ring system before bridging is fewer than two]

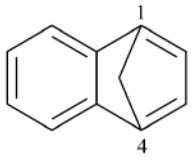
P-44.2.2.2.4.4 The senior bridged fused ring system is the bridged ring system with the senior fused ring system before bridging according to P-44.2.2.2.3 [criterion (d) in P-44.2.2.2.4].

Example (the symbol > means 'is senior to'):



4,7-methanoazulene (PIN)

>

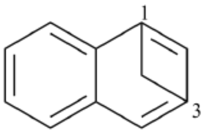


1,4-methanonaphthalene (PIN)

[azulene is senior to naphthalene, see P-44.2.1]

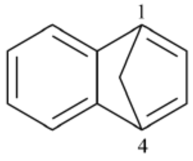
P-44.2.2.2.4.5 The senior bridged fused ring system has the lower set of locants for bridge attachments [criterion (e) in P-44.2.2.2.4].

Example (the symbol > means 'is senior to'):



1,3-methanonaphthalene (PIN)

>

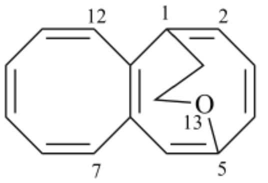


1,4-methanonaphthalene (PIN)

[the locant set for bridge attachments '1,3' is lower than '1,4']

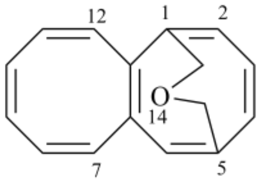
P-44.2.2.2.4.6 The senior bridged fused ring system has the lower locant(s) for heteroatoms in bridges, without regard to kind [criterion (f) in P-44.2.2.2.4].

Example (the symbol > means 'is senior to'):



5,1-(epoxyethano)octalene (PIN)

>

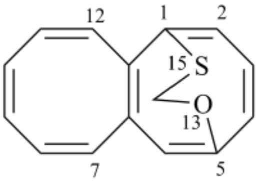


1,5-(methanooxymethano)octalene (PIN)

[the locant '13' for the bridge oxygen atom is lower than '14']

P-44.2.2.2.4.7 The senior bridged fused ring system has the lower locants for heteroatoms in bridges, in the order: F > Cl > Br > I > O > S > Se > Te > N > P > As > Sb > Bi > Si > Ge > Sn > Pb > B > Al > Ga > In > Tl [criterion (g) in P-44.2.2.2.4].

Example (the symbol > means 'is senior to'):



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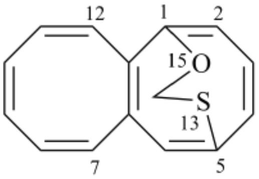


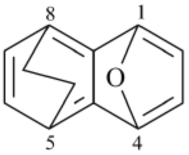
5,1-(epoxymethanosulfano)octalene (PIN)

1,5-(epoxymethanosulfano)octalene (PIN)

[the locant '13' for the senior oxygen atom in the bridge is lower than '15']

P-44.2.2.2.4.8 The senior bridged fused ring system has the fewer composite bridges [criterion (h) in P-44.2.2.2.4].

Example (the symbol > means 'is senior to'):



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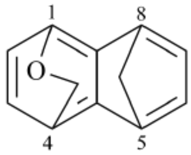


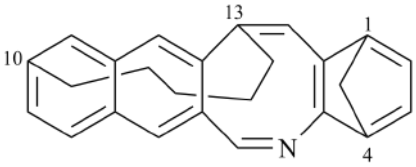
1,4-epoxy-5,8-ethanonaphthalene (PIN)

1,4-(epoxymethano)-5,8-methanonaphthalene (PIN)

[zero composite bridges is fewer than one]

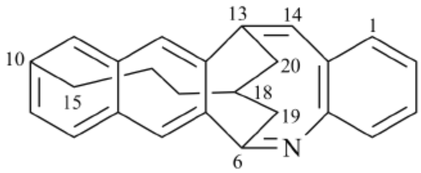
P-44.2.2.2.4.9 The senior bridged fused ring system has the fewer dependent bridges [criterion (i) in P-44.2.2.2.4].

Example (the symbol > means 'is senior to'):



(I)

>

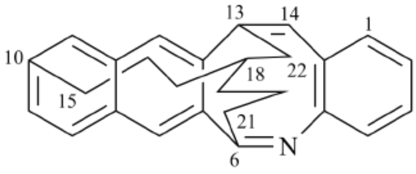


(II)

(**I**) 1,4-methano-10,13-pentanonaphtho[2,3-*c*][1]benzazocine (PIN)
is senior to
(**II**) 13,18-methano-6,10-pentanonaphtho[2,3-*c*][1]benzazocine (PIN)
[zero dependent bridges is fewer than one]

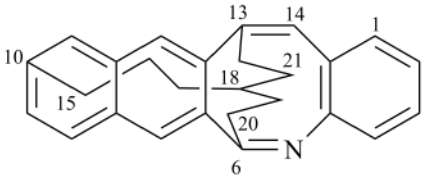
P-44.2.2.2.4.10 The senior bridged fused ring system has fewer atoms in dependent bridges [criterion (j) in P-44.2.2.2.4].

Example (the symbol > means 'is senior to'):



(I)

>

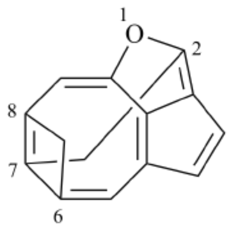


(II)

(**I**) 13,18-methano-6,10-heptanonaphtho[2,3-*c*][1]benzazocine (PIN)
is senior to
(**II**) 13,18-ethano-6,10-hexanonaphtho[2,3-*c*][1]benzazocine (PIN)
[one atom in the dependent bridge in (**I**) (atom 22)
is fewer the two atoms in (**II**) (atoms 21 and 22)]

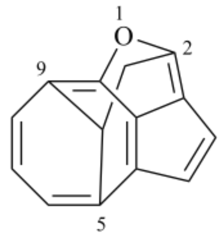
P-44.2.2.2.4.11 The senior bridged fused ring system has the greater number of divalent bridges [criterion (k) in P-44.2.2.2.4].

Example (the symbol > means 'is senior to'):



(**I**)

>

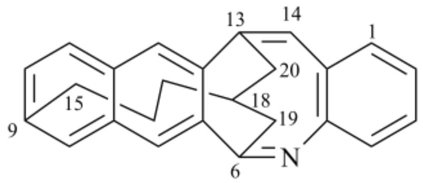


(**II**)

(**I**) 1-oxa-2,7:6,8-dimethanocycloocta[1,2,3-*cd*]pentalene (PIN)
is senior to
(**II**) 1-oxa-5,9,2-(ethane[1,1,2]triyl)cycloocta[1,2,3-*cd*]pentalene (PIN)
['2' divalent bridges in (**I**) is senior to the '1' trivalent bridge in (**II**)]

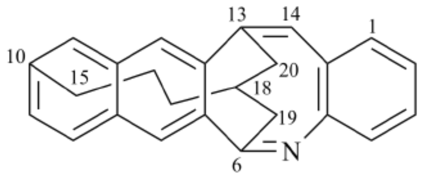
P-44.2.2.2.4.12 The senior bridged fused ring system has the lower set of locants for attachment of independent bridges [criterion (l) in P-44.2.2.2.4].

Example (the symbol > means 'is senior to'):



(**I**)

>

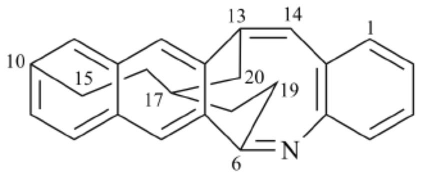


(**II**)

(**I**) 13,18-methano-6,9-pentanonaphtho[2,3-*c*][1]benzazocine (PIN)
is senior to
(**II**) 13,18-methano-6,10-pentanonaphtho[2,3-*c*][1]benzazocine (PIN)
[the locant set '6,9' for the independent bridge in (**I**) is lower than the locant set '6,10' in (**II**)]

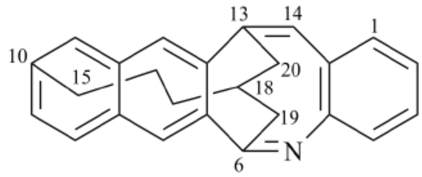
P-44.2.2.2.4.13 The senior bridged fused ring system has the lower set of locants for attachment of dependent bridges [criterion (m) in P-44.2.2.2.4].

Example (the symbol > means 'is senior to'):



(**I**)

>

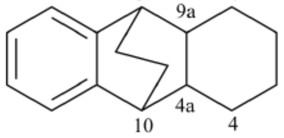


(**II**)

13,17-methano-6,10-pentanonaphtho[2,3-*c*][1]benzazocine (PIN) (**I**)
is senior to
13,18-methano-6,10-pentanonaphtho[2,3-*c*][1]benzazocine (PIN) (**II**)
[the locant set '13,17' for the dependent bridge in (**I**)
is lower than the locant set '13,18' in (**II**)]

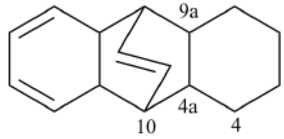
P-44.2.2.2.4.14 The senior bridged fused ring system has the fused ring system with the greater number of noncumulative double bonds before bridging [criterion (n) in P-44.2.2.2.4].

Example (the symbol > means 'is senior to'):



(**I**)

>



(**II**)

1,2,3,4,4a,9,9a,10-octahydro-9,10-ethanoanthracene (PIN) (**I**)
is senior to
1,2,3,4,4a,8a,9,9a,10,10a-decahydro-9,10-ethenoanthracene (PIN) (**II**)
[three noncumulative double bonds in (**I**) is greater than the
two noncumulative double bonds in (**II**)]

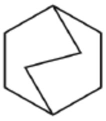
P-44.2.2.2.5 Seniority criteria for bridged nonfused ring systems (von Baeyer ring systems) are applied successively until there are no alternatives remaining. These criteria are illustrated in P-44.2.2.2.5.1 through P-44.2.2.2.5.3. The senior bridged nonfused ring system:

(a) has the lower number at the first point of difference in the descriptor set for describing ring sizes when considered in order of citation in the name;
(b) has the lower set of bridge attachment locants (superscript locants) at the first point of difference when compared term by term in order of increasing numerical value;
(c) has the lower set of bridge attachment locants (superscript locants) at first point of difference when compared term by term in their order of citation in the name.

Further criteria applicable to bridged nonfused ring systems are found in P-44.4.

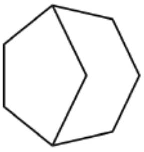
P-44.2.2.2.5.1 The senior bridged nonfused ring system has the lower number in the descriptor set for describing ring sizes at the first point of difference when considered in order of citation in the name [criteria (a) in P-44.2.2.2.5].

Example (the symbol > means 'is senior to'):



bicyclo[2.2.2]octane (PIN)

>

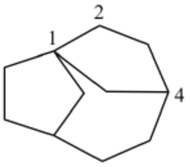


bicyclo[3.2.1]octane (PIN)

[the ring descriptor set '2,2,2' is lower than '3,2,1']

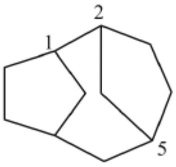
P-44.2.2.2.5.2 The senior bridged nonfused ring system has the lower set of bridge attachment locants (superscript locants) at the first point of difference when compared term by term in order of increasing numerical value [criteria (b) in P-44.2.2.2.5].

Example (the symbol > means 'is senior to'):



tricyclo[5.2.1.1^{1,4}]undecane (PIN)

>

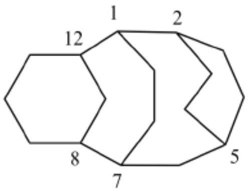


tricyclo[5.2.1.1^{2,5}]undecane (PIN)

[the bridge attachment locant set '1,4' is lower than '2,5']

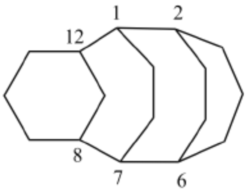
P-44.2.2.2.5.3 The senior bridged nonfused ring system has the lower set of bridge attachment locants (superscript locants) at first point of difference when compared term by term in their order of citation in the name [criterion (c) in P-44.2.2.2.5].

Example (the symbol > means 'is senior to'):



tetracyclo[5.5.2.2^{2,5}.1^{8,12}]heptadecane (PIN)

>



tetracyclo[5.5.2.2^{2,6}.1^{8,12}]heptadecane (PIN)

[the bridge attachment locant set '2,5,8,12' is lower than '2,6,8,12']

P-44.2.2.2.6 Linear (acyclic) phanes

Although linear phane systems can be viewed as heteroacyclic chains, in which the amplificants are heteroatoms and the connecting atoms or chains are carbon atoms, seniority for linear (acyclic) phanes follows closely the criteria used for cyclic phane systems (see P-44.2.2.2.2). Accordingly, the seniority criteria for linear phane systems given below are applied successively until no alternatives remain. These criteria are illustrated in P-44.2.2.2.6.1 through P-44.2.2.2.6.10. The senior linear phane system has:

(a) the senior amplificant, as defined by P-44.2.1.2 through P-44.2.1.8;
(b) most amplificants in their order of seniority as defined by P-44.2.1.2 through P-44.2.1.8;
(c) the maximum number of skeletal nodes;
(d) the lower superatom locant(s) for the senior amplificant;

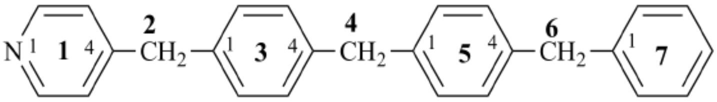
(e) the lower superatom locant(s) for all amplificants as a set when compared term by term in order of increasingvalue and then in order of citation in the name;
(f) the lower superatom locant(s) for all amplificants when compared in order of citation in the name;
(g) the lower set of attachment locants considered as a set when compared term by term in order of increasing numerical value;
(h) the lower set of attachment locants when compared term by term in their order of citation in the name;
(i) the greater number of heteroatoms introduced by skeletal replacement ('a') nomenclature without regard to kind;
(j) the greater number of heteroatoms introduced by skeletal replacement ('a') nomenclature first cited in the following order: F > Cl > Br > I > O > S > Se > Te > N > P > As > Sb > Bi > Si > Ge > Sn > Pb > B > Al > Ga > In > Tl.

Further criteria applicable to linear (acyclic) phanes are found in P-44.4.

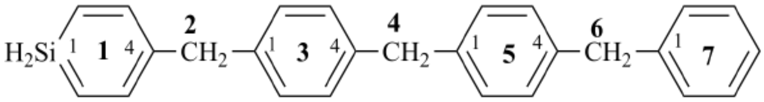
P-44.2.2.2.6.1 The senior linear phane system has the senior amplificant, as defined by P-44.2.1.2. through P-44.2.1.8 [criterion (a) in P-44.2.2.2.6]

Examples:

(1)

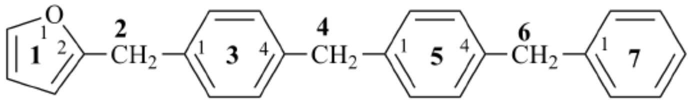


1(4)-pyridina-3,5(1,4),7(1)-tribenzenaheptaphane (PIN)
is senior to

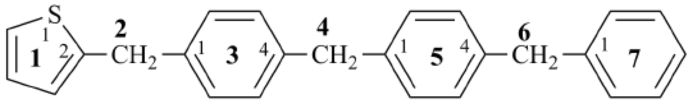


1(4)-silina-3,5(1,4),7(1)-tribenzenaheptaphane (PIN)
[the amplificant 'pyridina' is senior to the amplificant 'silina']

(2)

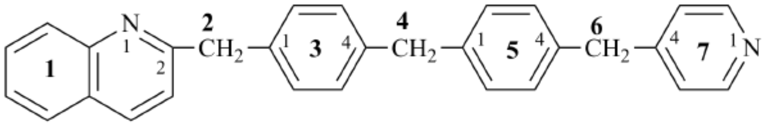


1(2)-furana-3,5(1,4),7(1)-tribenzenaheptaphane (PIN)
is senior to

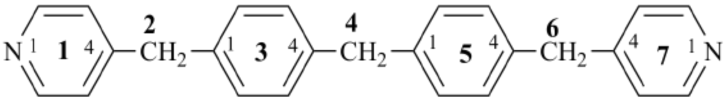


1(2)-thiophena-3,5(1,4),7(1)-tribenzenaheptaphane (PIN)
[the amplificant 'furana' is senior to the amplificant 'thiophena']

(3)

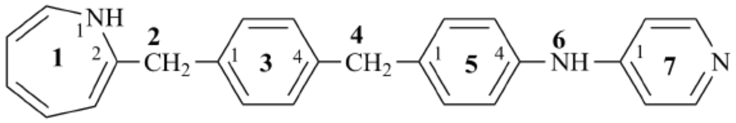


1(2)-quinolina-7(4)-pyridina-3,5(1,4)-dibenzenaheptaphane (PIN)
is senior to

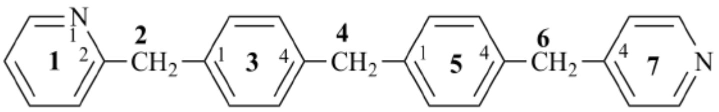


1,7(4)-dipyridina-3,5(1,4)-dibenzenaheptaphane (PIN)
[the amplificant 'quinolina' is senior to the amplificant 'pyridina']

(4)



1^1H-1(2)-azepina-7(4)-pyridina-3,5(1,4)-dibenzenaheptaphane (PIN)
is senior to

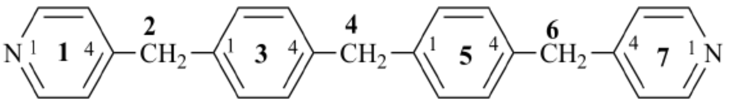


1(2),7(4)-dipyridina-3,5(1,4)-dibenzenaheptaphane (PIN)
[the amplificant 'azepina' is senior to the amplificant 'pyridina']

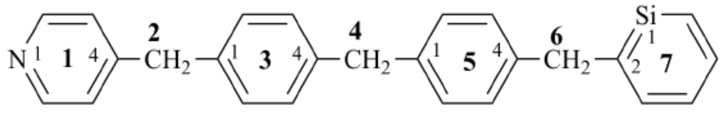
P-44.2.2.2.6.2 The senior linear phane system has the most amplificants in their order of seniority as defined by P-44.2.1.2 through P-44.2.1.8 [criterion (b) in P-44.2.2.2.6].

Examples:

(1)

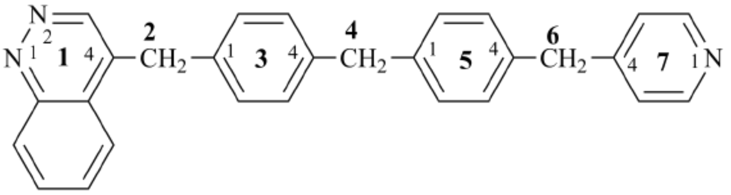

N
1
1
4
2
CH2
1
3
4
4
CH2
1
5
4
6
CH2
4
7
1
N

1,7(4)-dipyridina-3,5(1,4)-dibenzenaheptaphane (PIN)
is senior to

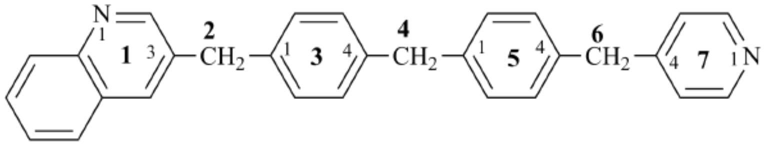

N
1
1
4
2
CH2
1
3
4
4
CH2
1
5
4
6
CH2
Si
1
2
7

1(4)-pyridina-7(2)-silina-3,5(1,4)-dibenzenaheptaphane (PIN)
[the amplificants ‘pyridina/pyridina’ are senior to the amplificants ‘pyridina/silina’]

(2)

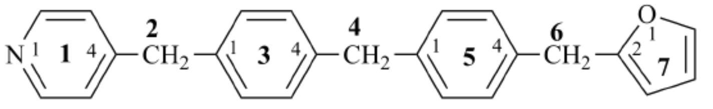

N
2
N
1
1
4
2
CH2
1
3
4
4
CH2
1
5
4
6
CH2
4
7
1
N

1(4)-cinnolina-7(4)-pyridina-3,5(1,4)-dibenzenaheptaphane (PIN)
is senior to

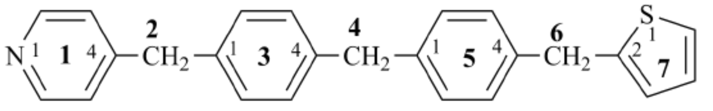

N
1
1
3
2
CH2
1
3
4
4
CH2
1
5
4
6
CH2
4
7
1
N

1(3)-quinolina-7(4)-pyridina-3,5(1,4)-dibenzenaheptaphane (PIN)
[the amplificants ‘cinnolina/pyridina’ are senior to the amplificants ‘quinolina/pyridina’]

(3)


N
1
1
4
2
CH2
1
3
4
4
CH2
1
5
4
6
CH2
O
1
2
7

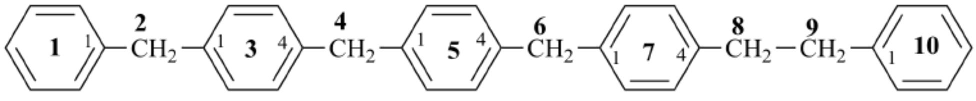
1(4)-pyridina-7(2)-furana-3,5(1,4)-dibenzenaheptaphane (PIN)
is senior to


N
1
1
4
2
CH2
1
3
4
4
CH2
1
5
4
6
CH2
S
1
2
7

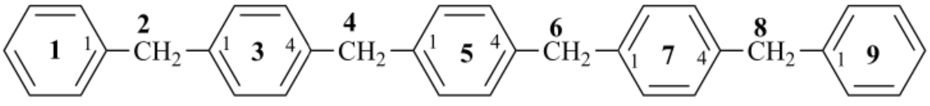
1(4)-pyridina-7(2)-thiophena-3,5(1,4)-dibenzenaheptaphane (PIN)
[the amplificants ‘pyridina/furana’ are senior to ‘pyridina/thiophena’]

P-44.2.2.2.6.3 The senior linear phane system has the maximum number of skeletal nodes [criterion (c) in P-44.2.2.2.6]

Example:


1
1
2
CH2
1
3
4
4
CH2
1
5
4
6
CH2
1
7
4
8
CH2
9
CH2
1
10

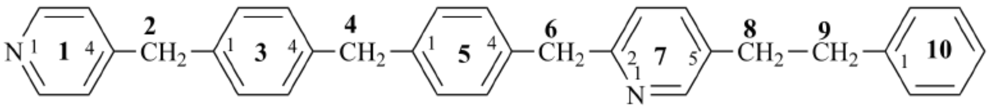
1,10(1),3,5,7(1,4)-pentabenzenadecaphane (PIN)
is senior to


1
1
2
CH2
1
3
4
4
CH2
1
5
4
6
CH2
1
7
4
8
CH2
1
9

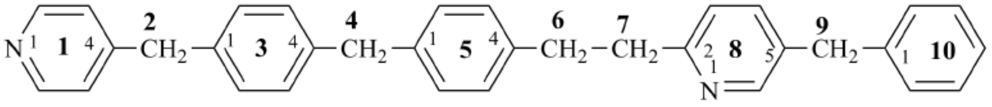
1,9(1),3,5,7(1,4)-pentabenzenanonaphane (PIN)
[the decaphane has more nodes than the nonaphane]

P-44.2.2.2.6.4 The senior linear phane system has the lower superatom locant(s) for the senior amplificants [criterion (d) in P-44.2.2.2.6].

Example:



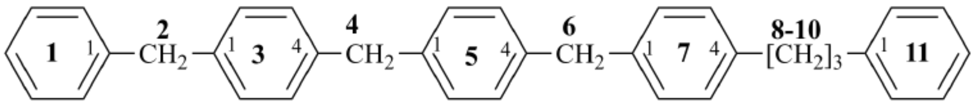
1(4),7(2,5)-dipyridina-3,5(1,4),10(1)-tribenzenadecaphane (PIN)
is senior to



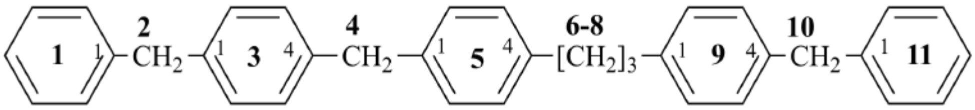
1(4),8(2,5)-dipyridina-3,5(1,4),10(1)-tribenzenadecaphane (PIN)
[the locant set ‘1,7’ for the pyridina amplificants is lower than the set ‘1,8’]

P-44.2.2.2.6.5 The senior linear phane system has the lower superatom locant(s) for all amplificants as a set when compared term by term in order of increasing seniority [criterion (e) in P-44.2.2.2.6].

Example:



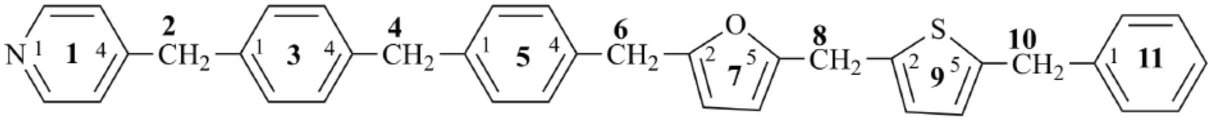
1,11(1),3,5,7(1,4)-pentabenzenaundecaphane (PIN)
is senior to



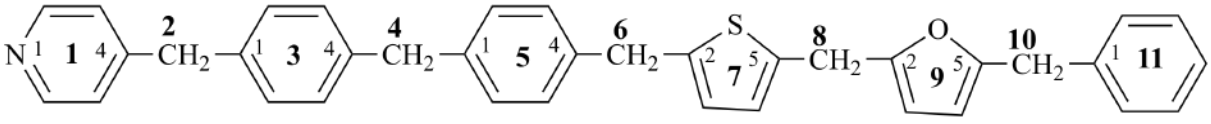
1,11(1),3,5,9(1,4)-pentabenzenaundecaphane (PIN)
[the locant set ‘1,3,5,7,11’ for the amplificants is lower than the set ‘1,3,5,9,11’]

P-44.2.2.2.6.6 The senior linear phane system has the lower superatom locant(s) for all amplificants when compared in order of citation in the name [criterion (f) in P-44.2.2.2.6].

Example:



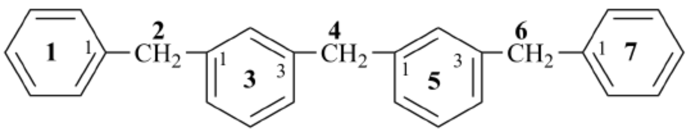
1(4)-pyridina-7(2,5)-furana-9(2,5)-thiophena-3,5(1,4),11(1)-tribenzenaundecaphane (PIN)
is senior to



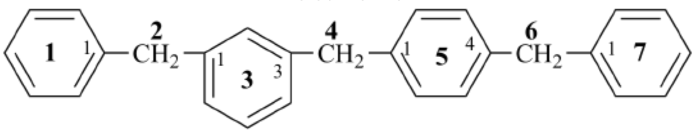
1(4)-pyridina-9(2,5)-furana-7(2,5)-thiophena-3,5(1,4),11(1)-tribenzenaundecaphane (PIN)
[the locant set for the amplificants in order of occurrence in
the name ‘1,7,9,3,5,11’ is lower than the locant set ‘1,9,7,3,5,11’]

P-44.2.2.2.6.7 The senior linear phane system has the lower set of attachment locants considered as a set when compared term by term in order of increasing numerical value [criterion (g) in P-44.2.2.2.6].

Example:



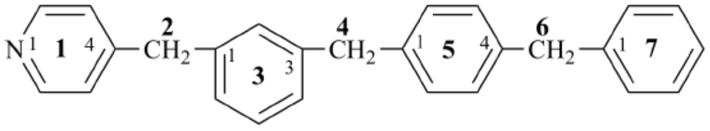
1,7(1),3,5(1,3)-tetrabenzenaheptaphane (PIN)
is senior to



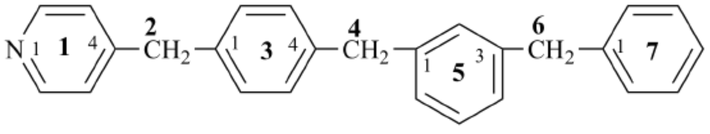
1,7(1),3(1,3),5(1,4)-tetrabenzenaheptaphane (PIN)
[the locant set ‘1,1,1,1,3,3’ for amplificant attachment locants in increasing numerical order is lower than ‘1,1,1,1,3,4’]

P-44.2.2.2.6.8 The senior linear phane system has the lower set of attachment locants when compared term by term in their order of citation in the name [criterion (h) in P-44.2.2.2.6].

Example:



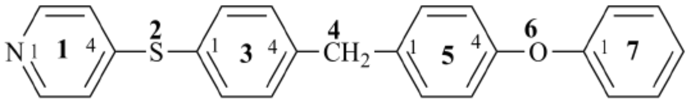
1(4)-pyridina-3(1,3),5(1,4),7(1)-tribenzenaheptaphane (PIN)
is senior to



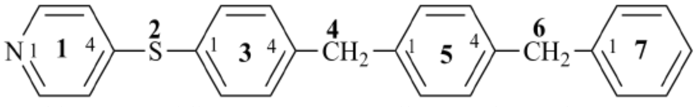
1(4)-pyridina-3(1,4),5(1,3),7(1)-tribenzenaheptaphane (PIN)
[the locant set ‘4,1,3,1,4,1’ for the amplificant locants in order of their citation in the name is lower than ‘4,1,4,1,3,1’]

P-44.2.2.2.6.9 The senior linear phane system has the greater number of heteroatoms introduced by skeletal replacement (‘a’) nomenclature without regard to kind [criterion (i) in P-44.2.2.2.6].

Example:



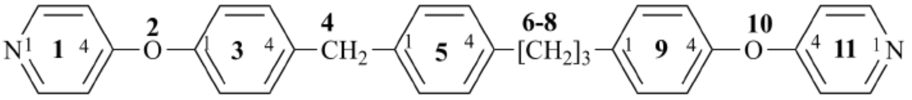
6-oxa-2-thia-1(4)-pyridina-3,5(1,4),7(1)-tribenzenaheptaphane (PIN)
is senior to



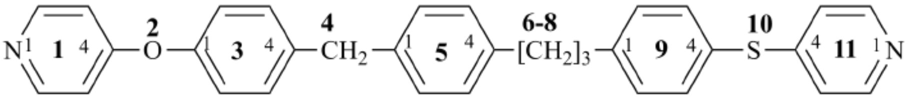
2-thia-1(4)-pyridina-3,5(1,4),7(1)-tribenzenaheptaphane (PIN)
[two heteroatoms intoduced by skeletal replacement (‘a’) nomenclature are senior to one such heteroatom]

P-44.2.2.2.6.10 The senior linear phane system has the greater number of heteroatoms introduced by skeletal replacement (‘a’) nomenclature first cited in the following order: F > Cl > Br > I > O > S > Se > Te > N > P > As > Sb > Bi > Si > Ge > Sn > Pb > B > Al > Ga > In > Tl [criterion (j) in P-44.2.2.2.6]

Example:



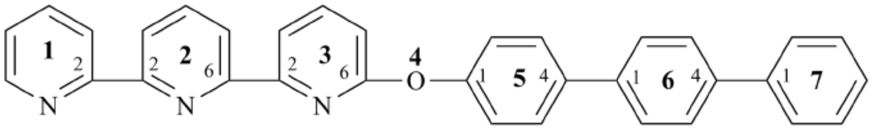
2,10-dioxa-1,11(4)-dipyridina-3,5,9(1,4)-tribenzenaundecaphane (PIN)
is senior to



2-oxa-10-thia-1,11(4)-dipyridina-3,5,9(1,4)-tribenzenaundecaphane (PIN)
[two oxygen atoms are senior to one oxygen atom and one sulfur atom]

P-44.2.2.2.7 Seniority criteria for ring assemblies are based on the appropriate criteria for rings and ring systems given in P-44.2.1. Phane nomenclature is used when two ring assemblies are linked together by atoms or chains to generate a system with at least seven nodes and two terminal rings or ring systems.

Example:



4-oxa-1(2),2,3(2,6)-tripyridina-5,6(1,4),7(1)-tribenzenaheptaphane (PIN)
1^6-([1^1,2^1:2^4,3^1]terphenyl]-1^4-yloxy)-1^2,2^2:2^6,3^2-terpyridine;
[criteria for phane nomenclature (see P-52.2.5.1) are met for the PIN]

The following rules for seniority of ring assemblies are applied successively until there are no alternatives remaining:

(a) rings containing any heteroatom;

(b) rings containing nitrogen;

(c) in the absence of nitrogen, rings containing at least one heteroatom first cited in the following sequence; F > Cl > Br > I > O > S > Se > Te > P > As > Sb > Bi > Si > Ge > Sn > Pb > B > Al > Ga > In > Tl;

(d) the greater number of rings;

(e) the greater number of atoms;

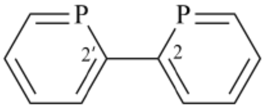
(f) the greater number of heteroatoms of any kind;

(g) the greater number of heteroatoms first cited in the following sequence: F > Cl > Br > I > O > S > Se >Te > N > P > As > Sb > Bi > Si > Ge > Sn > Pb > B > Al > Ga > In > Tl.

Further criteria applicable to ring assemblies are found in P-44.4.

P-44.2.2.2.7.1 The senior ring assembly is composed of rings containing any heteroatom [criterion (a) in P-44.2.2.2.7].

Example (the symbol > means 'is senior to'):



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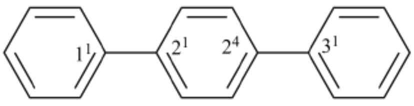
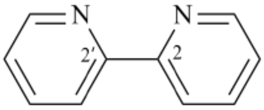


2,2′-biphosphinine (PIN)

1^1,2^1:2^4,3^1-terphenyl (PIN)
1,1′:4′,1″-terphenyl

P-44.2.2.2.7.2 The senior ring assembly is composed of rings containing nitrogen [criterion (b) in P-44.2.2.2.7].

Example (the symbol > means 'is senior to'):



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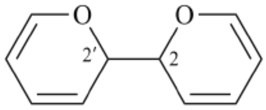
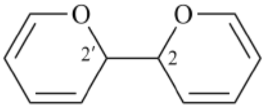


2,2′-bipyridine (PIN)

2*H*,2′*H*-2,2′-bipyran (PIN)

P-44.2.2.2.7.3 The senior ring assembly in the absence of nitrogen is composed of rings containing at least one hetero atom first cited in the following sequence: F > Cl > Br > I > O > S > Se >Te > P > As > Sb > Bi > Si > Ge > Sn > Pb > B > Al > Ga > In > Tl [criterion (c) in P-44.2.2.2.7].

Example (the symbol > means 'is senior to'):



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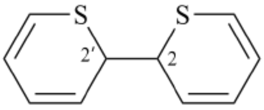


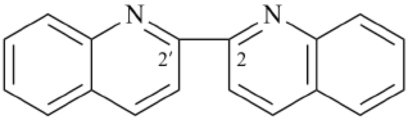
2*H*,2′*H*-2,2′-bipyran (PIN)

2*H*,2′*H*-2,2′-bithiopyran (PIN)

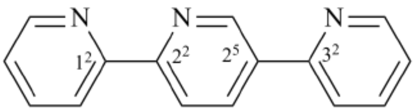
[one oxygen atom per ring is preferred to one sulfur atom per ring]

P-44.2.2.2.7.4 The senior ring assembly is composed of the greater number of rings [criterion (d) in P-44.2.2.2.7].

Example (the symbol > means 'is senior to'):



>



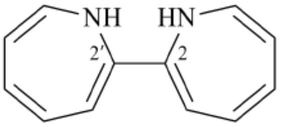
2,2′-biquinoline (PIN)

1^2,2^2:2^5,3^2-terpyridine (PIN)
2,2′:5′,2″-terpyridine

[a ring system consisting of two rings is senior to a ring system consisting of one ring]

P-44.2.2.2.7.5 The senior ring assembly is composed of the greater number of atoms [criterion (e) in P-44.2.2.2.7.]

Example (the symbol > means 'is senior to'):



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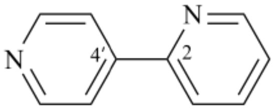


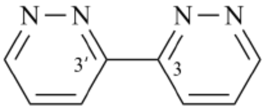
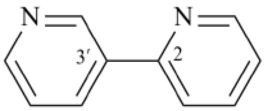
1*H*,1′*H*-2,2′-biazepine (PIN)

2,4′-bipyridine (PIN)

[seven atoms per ring is preferred to six atoms per ring]

P-44.2.2.2.7.6 The senior ring assembly is composed of the greater number of heteroatoms of any kind [criterion (f) in P-44.2.2.2.7].

Example (the symbol > means 'is senior to'):

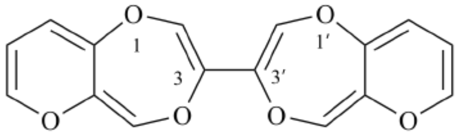
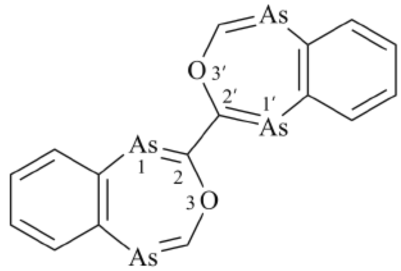

>


3,3′-bipyridazine (PIN) 2,3′-bipyridine (PIN)

[two heteroatoms per ring is preferred to one heteroatom per ring]

P-44.2.2.2.7.7 The senior ring assembly is composed of the greater number of heteroatoms in the order: F > Cl > Br > I > O > S > Se > Te > N > P > As > Sb > Bi > Si > Ge > Sn > Pb > B > Al > Ga > In > Tl [criterion(g)in P-44.2.2.2.7].

Example (the symbol > means ‘is senior to’):


>


3,3′-bipyrano[3,2-*e*][1,4]dioxepine (PIN) 2,2′-bi-3,1,5-benzoxadiarsepine (PIN)

[three oxygen atoms per ring preferred to one oxygen atom per ring]

P-44.3 SENIORITY OF ACYCLIC CHAINS (THE PRINCIPAL CHAIN)

In an acyclic compound consisting of individual atoms, alike or different (an acyclic chain), the chain on which the nomenclature and numbering is based is called the ‘principal chain’. When there is a choice for the principal chain, the following criteria are applied, in the order listed, until a decision is reached.

The principal chain:

(a) contains the greater number of heteroatoms of any kind;

(b) has the greater number of skeletal atoms;

(c) contains the greater number of the most senior acyclic heteroatom in the following sequence: O > S > Se > Te > N > P > As > Sb > Bi > Si > Ge > Sn > Pb > B > Al > Ga > In >Tl.

Each of these criteria is illustrated in P-44.3.1 through P-44.3.3 below.

Further criteria applicable to acyclic chains are found in P-44.4.

P-44.3.1 The principal chain contains the greater number of acyclic heteroatoms of any kind [criterion (a) in P-44.3].

Examples:

(1)

$$\overset{1}{CH_3}\text{-}\overset{2}{O}\text{-}CH_2\text{-}CH_2\text{-}\overset{5}{O}\text{-}CH_2\text{-}CH_2\text{-}\overset{8}{O}\text{-}CH_2\text{-}CH_2\text{-}\overset{11}{O}\text{-}CH_2\text{-}CH_2\text{-}\overset{14}{O}\text{-}CH_2\text{-}\overset{16}{CH_3}$$

2,5,8,11,14-pentaoxahexadecane (PIN)
is senior to

$$\overset{1}{CH_3}\text{-}\overset{2}{CH_2}\text{-}\overset{3}{O}\text{-}CH_2\text{-}CH_2\text{-}\overset{6}{O}\text{-}CH_2\text{-}CH_2\text{-}\overset{9}{O}\text{-}CH_2\text{-}CH_2\text{-}\overset{12}{O}\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}\overset{17}{CH_3}$$

3,6,9,12-tetraoxaheptadecane (PIN)
[five heteroatoms are greater than four]

(2)

$$\overset{1}{CH_3}\text{-}\overset{2}{SiH_2}\text{-}\overset{3}{CH_2}\text{-}CH_2\text{-}\overset{5}{SiH_2}\text{-}CH_2\text{-}CH_2\text{-}\overset{8}{SiH_2}\text{-}CH_2\text{-}CH_2\text{-}\overset{11}{SiH_2}\text{-}CH_2\text{-}CH_2\text{-}\overset{14}{SiH_2}\text{-}\overset{15}{CH_3}$$

2,5,8,11,14-pentasilapentadecane (PIN)
is senior to

$$\overset{1}{CH_3}\text{-}\overset{2}{CH_2}\text{-}\overset{3}{O}\text{-}CH_2\text{-}CH_2\text{-}\overset{6}{S}\text{-}CH_2\text{-}CH_2\text{-}\overset{9}{S}\text{-}CH_2\text{-}CH_2\text{-}\overset{12}{O}\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}\overset{17}{CH_3}$$

3,12-dioxa-6,9-dithiaheptadecane (PIN)
[five heteroatoms are greater than four]

P-44.3.2 The principal chain has the greater number of skeletal atoms [criterion (b) in P-44.3].

In acyclic parent structures the order of seniority between unsaturation and length of chain given in earlier recommendations is reversed. Thus, the first criterion to be considered in choosing a preferred parent acyclic chain is the length of the chain; unsaturation is now the second criterion.

Example (the symbol > means ‘is senior to’):

(1) $\overset{1}{C}H_3\text{-}\overset{2}{C}H_2\text{-}\overset{3}{C}H_2\text{-}\overset{4}{C}H_2\text{-}\overset{5}{C}H_3$ > $\overset{1}{C}H_3\text{-}\overset{2}{C}H_2\text{-}\overset{3}{C}H_2\text{-}\overset{4}{C}H_3$

pentane (PIN) butane (PIN)

[five skeletal atoms is greater than four]

(2) $\overset{1}{Si}H_3\text{-}\overset{2}{Si}H_2\text{-}\overset{3}{Si}H_2\text{-}\overset{4}{Si}H_2\text{-}\overset{5}{Si}H_3$ > $\overset{1}{Si}H_3\text{-}\overset{2}{Si}H_2\text{-}\overset{3}{Si}H_2\text{-}\overset{4}{Si}H_3$

pentasilane (preselected name; see P-12.2) tetrasilane (preselected name; see P-12.2)

[five skeletal atoms is greater than four)]

(3) $\overset{1}{C}H_3\text{-}\overset{2}{C}H_2\text{-}\overset{3}{C}H_2\text{-}\overset{4}{C}H_2\text{-}\overset{5}{C}H_2\text{-}\overset{6}{C}H_2\text{-}\overset{7}{C}H_2\text{-}\overset{8}{C}H_3$ > $\overset{1}{C}H_2{=}\overset{2}{C}H\text{-}\overset{3}{C}H_2\text{-}\overset{4}{C}H_2\text{-}\overset{5}{C}H_2\text{-}\overset{6}{C}H_2\text{-}\overset{7}{C}H_3$

octane (PIN) hept-1-ene (PIN)

[eight skeletal atoms is greater than seven]

(4) $\overset{13}{C}H_3\text{-}\overset{12}{C}H_2\text{-}\overset{11}{C}H_2\text{-}\overset{10}{C}H_2\text{-}\overset{9}{C}H_2\text{-}\overset{8}{C}H_2\text{-}\overset{7}{C}H_2\text{-}\overset{6}{C}H_2\text{-}\overset{5}{C}H_2\text{-}\overset{4}{C}H{=}\overset{3}{C}H\text{-}\overset{2}{C}H{=}\overset{1}{C}H_2$

trideca-1,3-diene (PIN)
is senior to

$\overset{8}{C}H_3\text{-}\overset{7}{C}H{=}\overset{6}{C}{=}\overset{5}{C}H\text{-}\overset{4}{C}H{=}\overset{3}{C}H\text{-}\overset{2}{C}H{=}\overset{1}{C}H_2$

octa-1,3,5,6-tetraene (PIN)
[thirteen skeletal atoms is greater than eight]

(5) $\overset{1}{C}H_3\text{-}\overset{2}{C}H_2\text{-}\overset{3}{O}\text{-}CH_2\text{-}CH_2\text{-}\overset{6}{O}\text{-}CH_2\text{-}CH_2\text{-}\overset{9}{O}\text{-}CH_2\text{-}CH_2\text{-}\overset{12}{O}\text{-}CH_2\text{-}CH_2\text{-}\overset{15}{C}H_3$

3,6,9,12-tetraoxapentadecane (PIN)
is senior to

$\overset{1}{C}H_3\text{-}\overset{2}{C}H_2\text{-}\overset{3}{O}\text{-}CH_2\text{-}CH_2\text{-}\overset{6}{O}\text{-}CH_2\text{-}CH_2\text{-}\overset{9}{O}\text{-}CH_2\text{-}CH_2\text{-}\overset{12}{O}\text{-}CH_2\text{-}\overset{14}{C}H_3$

3,6,9,12-tetraoxatetradecane (PIN)
[four heteroatoms in each chain and fifteen skeletal atoms is greater than fourteen]

(6) $\overset{1}{C}H_3\text{-}\overset{2}{Si}H_2\text{-}\overset{3}{C}H_2\text{-}CH_2\text{-}\overset{5}{Si}H_2\text{-}CH_2\text{-}CH_2\text{-}\overset{8}{Si}H_2\text{-}CH_2\text{-}CH_2\text{-}\overset{11}{Si}H_2\text{-}CH_2\text{-}\overset{13}{C}H_3$

2,5,8,11-tetrasilatridecane (PIN)
is senior to

$\overset{1}{Si}H_3\text{-}\overset{2}{Si}H_2\text{-}\overset{3}{Si}H_2\text{-}\overset{4}{Si}H_3$

tetrasilane (preselected name; see P-12.2)
[four heteroatoms in each chain and thirteen skeletal atoms is greater than four]

(7) $\overset{1}{C}H_3\text{-}\overset{2}{Si}H_2\text{-}\overset{3}{C}H_2\text{-}CH_2\text{-}\overset{5}{Si}H_2\text{-}CH_2\text{-}CH_2\text{-}\overset{8}{Si}H_2\text{-}CH_2\text{-}CH_2\text{-}\overset{11}{Si}H_2\text{-}CH_2\text{-}CH_2\text{-}\overset{14}{Si}H_2\text{-}\overset{15}{C}H_3$

2,5,8,11,14-pentasilapentadecane (PIN)
is senior to

$SiH_3\text{-}O\text{-}SiH_2\text{-}O\text{-}SiH_3$

trisiloxane (preselected name; see P-12.2)
[five heteroatoms in each chain; and fifteen skeletal atoms greater than five]

P-44.3.3 The principal chain contains the greater number of the most senior acyclic heteroatom in the order: O > S > Se > Te > N > P > As > Sb > Bi > Si > Ge > Sn > Pb > B > Al > Ga > In >Tl [criterion (c) in P-44.3].

Example (the symbol > means ‘is senior to’):

(1) $\overset{1}{C}H_3\text{-}\overset{2}{O}\text{-}\overset{3}{C}H_2\text{-}CH_2\text{-}\overset{5}{O}\text{-}CH_2\text{-}CH_2\text{-}\overset{8}{O}\text{-}CH_2\text{-}CH_2\text{-}\overset{11}{O}\text{-}CH_2\text{-}\overset{13}{C}H_3$

2,5,8,11-tetraoxatridecane (PIN)

is senior to

$\overset{1}{C}H_3\text{-}\overset{2}{O}\text{-}\overset{3}{C}H_2\text{-}CH_2\text{-}\overset{5}{O}\text{-}CH_2\text{-}CH_2\text{-}\overset{8}{O}\text{-}CH_2\text{-}CH_2\text{-}\overset{11}{S}\text{-}CH_2\text{-}\overset{13}{C}H_3$

2,5,8-trioxa-11-thiatridecane (PIN)
[four oxygen atoms is more than three]

(2) $SiH_3\text{-}O\text{-}SiH_3$ > $SiH_3\text{-}S\text{-}SiH_3$
disiloxane (preselected name; see P-12.2) > disilathiane (preselected name; see P-12.2)

[oxygen is senior to sulfur]

(3) $SiH_3\text{-}O\text{-}SiH_3$ > $SiH_3\text{-}SiH_2\text{-}SiH_3$
disiloxane (preselected name; see P-12.2) > trisilane (preselected name; see P-12.2)

[oxygen is senior to silicon]

P-44.4 SENIORITY CRITERIA APPLICABLE TO RINGS, RING SYSTEMS, OR ACYCLIC CHAINS

P-44.4.1 If the criteria of P-44.1 through P-44.3, where applicable, do not effect a choice of a senior parent structure, the following criteria are applied successively until there are no alternatives remaining. These criteria are illustrated in P-44.4.1.1 through P-44.4.1.12.

The senior ring, ring system, or principal chain:

(a) has the greater number of multiple bonds (P-44.4.1.1);

(b) has the greater number of double bonds (P-44.4.1.2);

(c) has one or more atoms with nonstandard bonding numbers (P-44.4.1.3);

(d) has the lower locants for indicated hydrogen (P-44.4.1.4);

(e) has the lower locants for heteroatoms introduced by skeletal replacement (‘a’) nomenclature as a set (P-44.4.1.5);

(f) has lower locants for heteroatoms introduced by skeletal replacement (‘a’) nomenclature in the order: F > Cl > Br > I > O > S > Se > Te > N > P > As > Sb > Bi > Si > Ge > Sn > Pb > B > Al > Ga > In > Tl (P-44.4.1.6);

(g) has the lower locant(s) for carbon atoms at fusion sites (P-44.4.1.7);

(h) has the lower locant for an attached group expressed as a suffix (P-44.4.1.8);

(i) has the lower locants for points of attachment (if a substituent group) (P-44.4.1.9);

(j) has the lower locant(s) for endings or prefixes that express changes in the level of hydrogenation, i.e., for ‘ene’ and ‘yne’ endings and ‘hydro/dehydro’ prefixes (P-44.4.1.10);

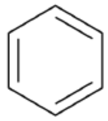
(k) has one or more isotopically modified atoms (P-44.4.1.11);

(l) has one or more stereogenic centers (P-44.4.1.12).

P-44.4.1.1 The senior ring, ring system or principal chain has the greater number of multiple bonds; for the purpose of this criterion, mancude rings or ring systems are considered as consisting of noncumulative double bonds [criterion (a) in P-44.4.1].

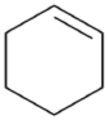
Example (the symbol > means ‘is senior to’):

(1)



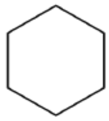
benzene (PIN)

>



cyclohexene (PIN)

>



cyclohexane (PIN)

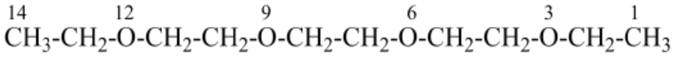
[two double bonds greater than one double bond that is greater than zero]

(2) $\overset{5}{C}H_3\text{-}\overset{4}{C}H{=}\overset{3}{C}H\text{-}\overset{2}{C}{\equiv}\overset{1}{C}H$ > $\overset{5}{C}H_3\text{-}\overset{4}{C}H_2\text{-}\overset{3}{C}H{=}\overset{2}{C}H\text{-}\overset{1}{C}H_3$
pent-3-en-1-yne (PIN) > pent-2-ene (PIN)

[two multiple bonds greater than one]

(3) $\overset{14}{C}H_3\text{-}CH_2\text{-}\overset{12}{O}\text{-}CH_2\text{-}CH_2\text{-}\overset{9}{O}\text{-}CH_2\text{-}CH_2\text{-}\overset{6}{O}\text{-}CH_2\text{-}CH_2\text{-}\overset{3}{O}\text{-}CH{=}\overset{1}{C}H$

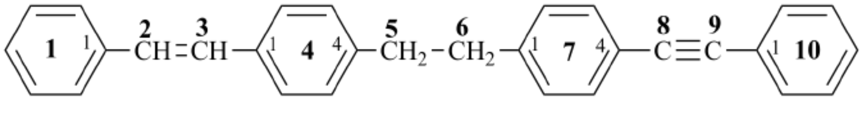
3,6,9,12-tetraoxatetradec-1-ene (PIN)
is senior to



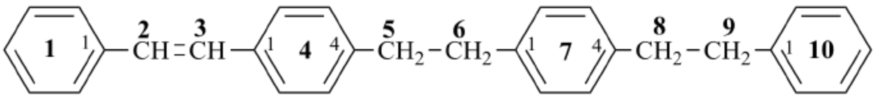
$\overset{14}{CH_3}\text{-}CH_2\text{-}\overset{12}{O}\text{-}CH_2\text{-}CH_2\text{-}\overset{9}{O}\text{-}CH_2\text{-}CH_2\text{-}\overset{6}{O}\text{-}CH_2\text{-}CH_2\text{-}\overset{3}{O}\text{-}\overset{1}{CH_2}\text{-}CH_3$

3,6,9,12-tetraoxatetradecane (PIN)
[one double bond greater than zero]

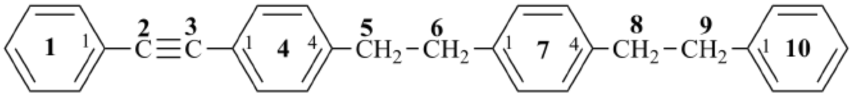
(4)



1,10(1),4,7(1,4)-tetrabenzenadecaphan-2-en-8-yne (PIN)
is senior to



1,10(1),4,7(1,4)-tetrabenzenadecaphan-2-ene (PIN)
[two multiple bonds senior to one multiple bond]
or to

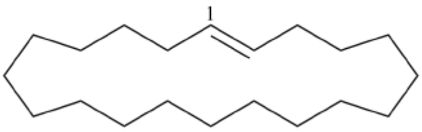


1,10(1),4,7(1,4)-tetrabenzenadecaphan-2-yne (PIN)
[one double bond senior to one triple bond]

P-44.4.1.2 The senior ring, ring system, or principal chain has the greater number of double bonds [criterion (b) in P-44.4.1].

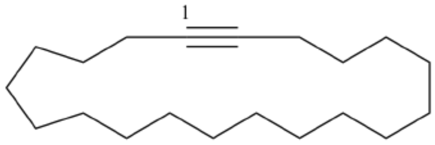
Example (the symbol > means 'is senior to'):

(1)



(*E*)-cycloicosene (PIN)

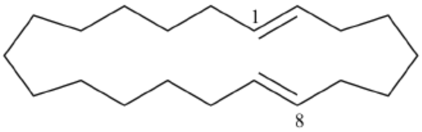
>



cycloicosyne (PIN)

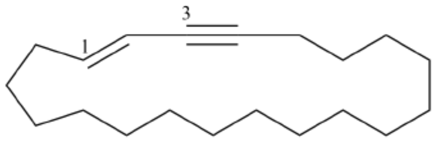
[one double bond is senior to one triple bond]

(2)



(1*E*,8*E*)-cycloicosa-1,8-diene (PIN)

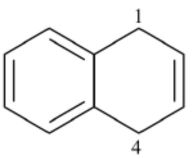
>



(1*E*)-cycloicos-1-en-3-yne (PIN)

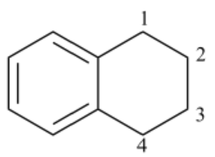
[two double bonds are senior to one double bond and one triple bond]

(3)



1,4-dihydronaphthalene (PIN)

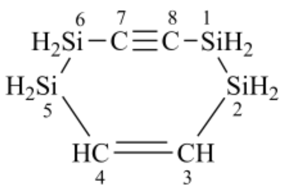
>



1,2,3,4-tetrahydronaphthalene (PIN)

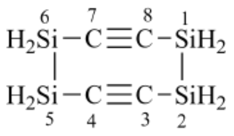
[four double bonds are greater than three]

(4)



1,2,5,6-tetrasilacyclooct-3-en-7-yne (PIN)

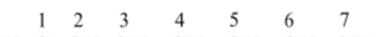
>



1,2,5,6-tetrasilacycloocta-3,7-diyne (PIN)

[one double bond and one triple bond is senior to two triple bonds
since a double bond is senior to a triple bond]

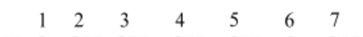
(5)



$\overset{1}{H_2C}\text{=}\overset{2}{CH}\text{-}\overset{3}{CH_2}\text{-}\overset{4}{CH_2}\text{-}\overset{5}{CH_2}\text{-}\overset{6}{CH}\text{=}\overset{7}{CH_2}$

hepta-1,6-diene (PIN)

>

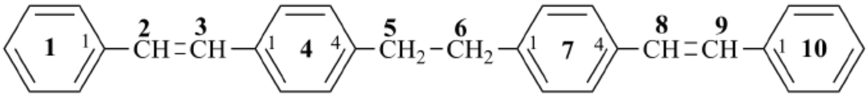


$\overset{1}{H_2C}\text{=}\overset{2}{CH}\text{-}\overset{3}{CH_2}\text{-}\overset{4}{CH_2}\text{-}\overset{5}{CH_2}\text{-}\overset{6}{C}\equiv\overset{7}{CH}$

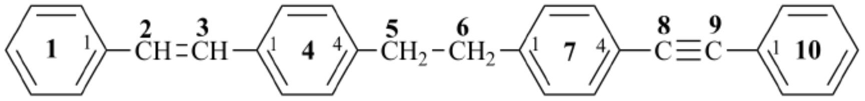
hept-1-en-6-yne (PIN)

[two double bonds are senior to one double bond and one triple bond
since a double bond is senior to a triple bond]

(6)



1,10(1),4,7(1,4)-tetrabenzenadecaphane-2,8-diene (PIN)
is senior to



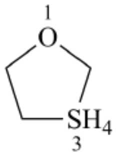
1,10(1),4,7(1,4)-tetrabenzenadecaphan-2-en-8-yne (PIN)
[two double bonds are senior to one double bond and
one triple bond since a double bond is senior to a triple bond]

P-44.4.1.3 The senior ring, ring system, or principal chain has one or more atoms with nonstandard bonding numbers [criterion (c) in P-44.4.1]. When choices are possible the following criteria are used in turn until a decision is reached.

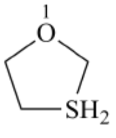
P-44.4.1.3.1 When a choice is needed between two chains or between two rings or ring systems having skeletal atoms with nonstandard bonding numbers, the one having the maximum number of atoms with nonstandard bonding numbers is chosen as principal chain or senior ring or ring system. If a further choice is needed between the same skeletal atom with different nonstandard bonding numbers, preference for the senior parent structure is given in order of the decreasing numerical value of the bonding number, i.e., λ^6 is senior to λ^4.

Example (the symbol > means 'is senior to'):

(1)



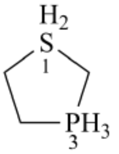
>



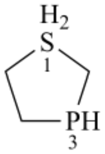
1,3λ^6-oxathiolane (PIN) 1,3λ^4-oxathiolane (PIN)

[the nonstandard bonding number λ^6 is senior to λ^4]

(2)



>



1λ^4,3λ^5-thiaphospholane (PIN) 1λ^4,3-thiaphospholane (PIN)

[two nonstandard bonding atoms greater than one]

(3) $\overset{1}{\mathrm{SiH_3}}\text{-}\overset{2}{\mathrm{SH_4}}\text{-}\overset{3}{\mathrm{SiH_3}}$ > $\overset{1}{\mathrm{SiH_3}}\text{-}\overset{2}{\mathrm{S}}\text{-}\overset{3}{\mathrm{SiH_3}}$

2λ^6-disilathiane
(preselected name; see P-12.2)

disilathiane
(preselected name; see P-12.2)

[the nonstandard bonding number λ^6 is senior to λ^2]

(4) $\overset{2}{\mathrm{PH_2}}\text{-}\overset{1}{\mathrm{PH_4}}$ > $\overset{2}{\mathrm{PH_2}}\text{-}\overset{1}{\mathrm{PH_2}}$

1λ^5-diphosphane
(preselected name; see P-12.2)

diphosphane
(preselected name; see P-12.2)

[the nonstandard bonding number λ^5 is senior to λ^3]

P-44.4.1.3.2 When a choice is needed between two chains or rings or ring systems having skeletal atoms with nonstandard bonding numbers, the one having the lowest locant(s) for (an) atom(s) with nonstandard bonding number(s) is chosen as principal chain or senior ring or ring system. If a further choice is needed, the one with the higher bonding number with the lowest locant is chosen.

Example (the symbol > means 'is senior to'):

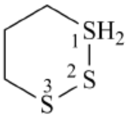
(1) $\overset{1}{\mathrm{H_3S}}\text{-}\overset{2}{\mathrm{S}}\text{-}\overset{3}{\mathrm{SH}}$ > $\overset{1}{\mathrm{HS}}\text{-}\overset{2}{\mathrm{SH_2}}\text{-}\overset{3}{\mathrm{SH}}$

1λ^4-trisulfane
(preselected name, see P-12.2)

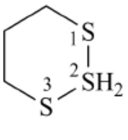
2λ^4-trisulfane
(preselected name, see P-12.2)

[the locant '1' for the atom with the nonstandard bonding number is lower than '2']

(2)



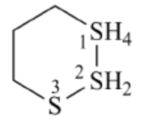
>



1λ^4,2,3-trithiane (PIN) 1,2λ^4,3-trithiane (PIN)

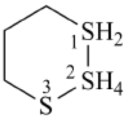
[the locant '1' for the atom with the nonstandard bonding number is lower than '2']

(3)



1 SH4
2 SH2
3 S

>



1 SH2
2 SH4
3 S

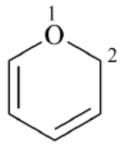
1λ^6,2λ^4,3-trithiane (PIN) 1λ^4,2λ^6,3-trithiane (PIN)

[the locant sets '1,2' for the atoms with the nonstandard bonding number are the same,'1,2' but the superscript arabic number set giving the actual nonstandard bonding state is compared and the number set '6,4' is senior to '4,6']

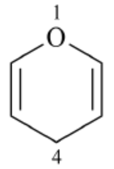
P-44.4.1.4 The senior ring or ring system has the lowest locants for indicated hydrogen [criterion (d) in P-44.4.1].

Example (the symbol > means 'is senior to'):

(1)



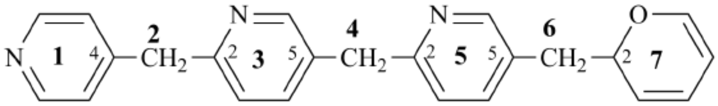
>



2H-pyran (PIN) *4H*-pyran (PIN)

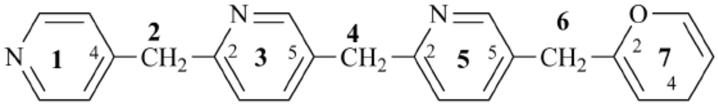
['*2H*' is lower than '*4H*']

(2)



N
1
4
2
CH2
N
2
3
5
4
CH2
N
2
5
5
6
CH2
O
2
7

$7^{2}H$-1(4),3,5(2,5)-tripyridina-7(2)-pyranaheptaphane (PIN)
is senior to



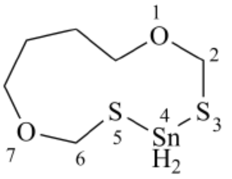
N
1
4
2
CH2
N
2
3
5
4
CH2
N
2
5
5
6
CH2
O
2
7
4

$7^{4}H$-1(4),3,5(2,5)-tripyridina-7(2)-pyranaheptaphane (PIN)
['$7^{2}H$' is lower than '$7^{4}H$']

P-44.4.1.5 The senior ring, ring system, or principal chain has the lower locants for heteroatoms introduced by skeletal replacement ('a') nomenclature as a set [criterion (e) in P-44.4.1].

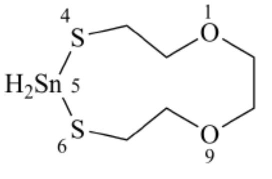
Example (the symbol > means 'is senior to'):

(1)



1
O
2
S
3
4
Sn
H2
S
5
6
O
7

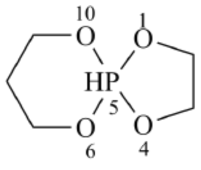
1,7-dioxa-3,5-dithia-4-stannacycloundecane (PIN)
is senior to



4
S
O
1
H2Sn 5
S
6
O
9

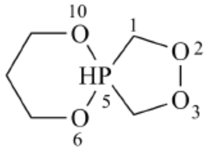
1,9-dioxa-4,6-dithia-5-stannacycloundecane (PIN)
[the heteroatom locant set '1,3,4,5,7' is lower than '1,4,5,6,9']

(2)



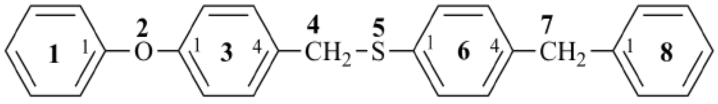
10
O
1
O
HP
5
O
6
O
4

1,4,6,10-tetraoxa-5λ^5-phosphaspiro[4.5]decane (PIN)
is senior to

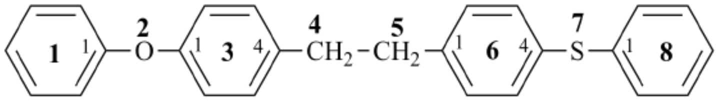


2,3,6,10-tetraoxa-5λ^5-phosphaspiro[4.5]decane (PIN)
[the heteroatom locant set ‘1,4,5,6,10’ is lower than ‘2,3,5,6,10’]

(3)

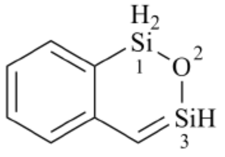


2-oxa-5-thia-1,8(1),3,6(1,4)-tetrabenzenaoctaphane (PIN)
is senior to

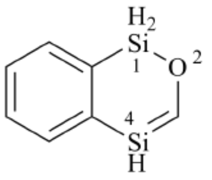


2-oxa-7-thia-1,8(1),3,6(1,4)-tetrabenzenaoctaphane (PIN)
[the heteroatom locant set ‘2,5’ is lower than ‘2,7’]

(4)



>

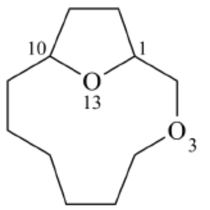


1*H*-2,1,3-benzoxadisiline (PIN)

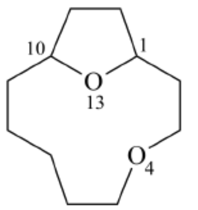
1*H*-2,1,4-benzoxadisiline (PIN)

[the heteroatom locant set ‘1,2,3’ is lower than ‘1,2,4’]

(5)



>



3,13-dioxabicyclo[8.2.1]tridecane (PIN)

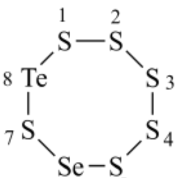
4,13-dioxabicyclo[8.2.1]tridecane (PIN)

[the heteroatom locant set ‘3,13’ is lower than ‘4,13’]

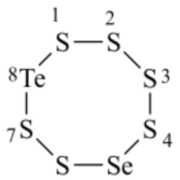
P-44.4.1.6 The senior ring, ring system, or principal chain has lower locants for heteroatoms introduced by skeletal replacement (‘a’) nomenclature in the order: F > Cl > Br > I > O > S > Se > Te > N > P > As > Sb > Bi > Si > Ge > Sn > Pb > B > Al > Ga > In > Tl [criterion (f) in P-44.4.1].

Example (the symbol > means ‘is senior to’):

(1)



>

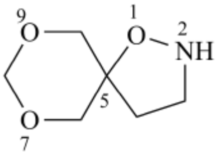


1,2,3,4,5,7,6,8-hexathiaselenatellurocane
(preselected name, see P-12.2)

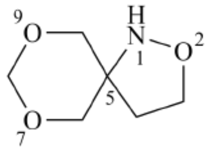
1,2,3,4,6,7,5,8-hexathiaselenatellurocane
(preselected name, see P-12.2)

[the heteroatom locant set ‘1,2,3,4,5,7,6,8’ is lower than ‘1,2,3,4,6,7,5,8’]

(2)



>

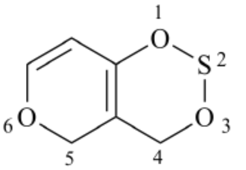


1,7,9-trioxa-2-azaspiro[4.5]decane (PIN)

2,7,9-trioxa-1-azaspiro[4.5]decane (PIN)

[the heteroatom locant set ‘1,7,9,2’ in the order of their citation in the name
is lower than ‘2,7,9,1’]

(3)



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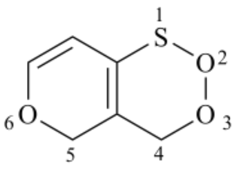
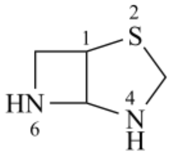


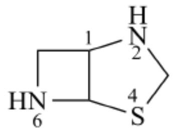
4*H*,5*H*-pyrano[4,3-*d*][1,3,2]dioxathiine (PIN) 4*H*,5*H*-pyrano[4,3-*d*][1,2,3]dioxathiine (PIN)

[the locant set ‘1,3,6’ for the senior oxygen atoms is lower than ‘2,3,6’]

(4)



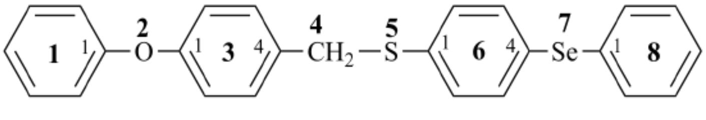
>



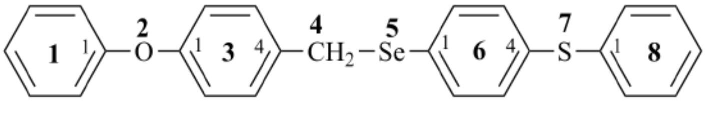
2-thia-4,6-diazabicyclo[3.2.0]heptane (PIN) 4-thia-2,6-diazabicyclo[3.2.0]heptane (PIN)

[the locant ‘2’ for the senior sulfur atom is lower than ‘4’]

(5)



2-oxa-5-thia-7-selena-1,8(1),3,6(1,4)-tetrabenzenaoctaphane (PIN)
is senior to

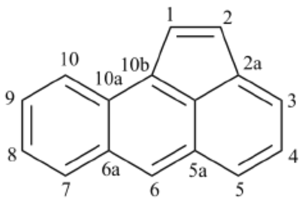


2-oxa-7-thia-5-selena-1,8(1),3,6(1,4)-tetrabenzenaoctaphane (PIN)
[the ‘S’ atom > the ‘Se’ at locant number ‘5’]

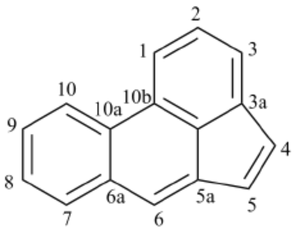
P-44.4.1.7 The senior fused ring system has the lower locant(s) for carbon atoms at fusion sites [criterion (g) in P-44.4.1].

Example (the symbol > means ‘is senior to’):

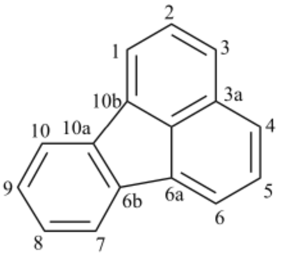
(1)



>



>

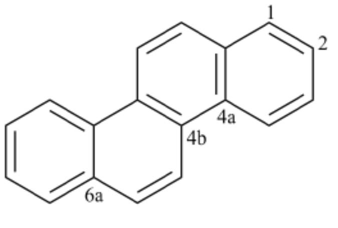


aceanthrylene (PIN) acephenanthrylene (PIN) fluoranthene (PIN)

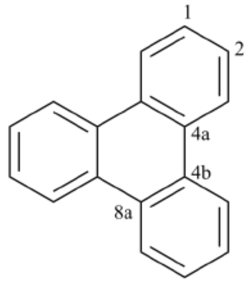
(I) **(II)** **(III)**

[the locant ‘2a’ for the fusion site in (**I**) is lower than ‘3a’ in (**II**) and
the locant set ‘3a,5a’ for the fusion sites in (**II**) is lower than ‘3a,6a’ in (**III**)]

(2)



>



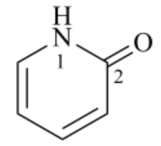
chrysene (PIN) triphenylene (PIN)

[the locant set ‘4a,4b,6a’ for the fusion sites is lower than ‘4a,4b,8a’]

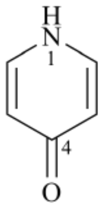
P-44.4.1.8 The senior ring, ring system, or principal chain has the lower locants for characteristic groups cited as a suffix [criterion (h) in P-44.4.1].

Example (the symbol > means ‘is senior to’):

(1)



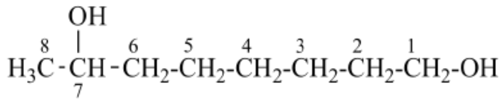
>



pyridin-2(1*H*)-one (PIN) pyridin-4(1*H*)-one (PIN)

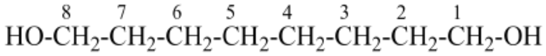
[the locant ‘2’ for the principal characteristic group is lower than ‘4’]

(2)



$$\overset{8}{\mathrm{H_3C}}\text{-}\underset{7}{\overset{\mathrm{OH}}{\mathrm{CH}}}\text{-}\overset{6}{\mathrm{CH_2}}\text{-}\overset{5}{\mathrm{CH_2}}\text{-}\overset{4}{\mathrm{CH_2}}\text{-}\overset{3}{\mathrm{CH_2}}\text{-}\overset{2}{\mathrm{CH_2}}\text{-}\overset{1}{\mathrm{CH_2}}\text{-OH}$$

octane-1,7-diol (PIN)
is senior to

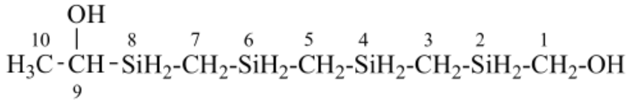


$$\text{HO-}\overset{8}{\mathrm{CH_2}}\text{-}\overset{7}{\mathrm{CH_2}}\text{-}\overset{6}{\mathrm{CH_2}}\text{-}\overset{5}{\mathrm{CH_2}}\text{-}\overset{4}{\mathrm{CH_2}}\text{-}\overset{3}{\mathrm{CH_2}}\text{-}\overset{2}{\mathrm{CH_2}}\text{-}\overset{1}{\mathrm{CH_2}}\text{-OH}$$

octane-1,8-diol (PIN)

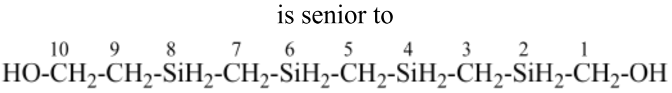
[(the locant set ‘1,7’ for the principal characteristic group is lower than ‘1,8’]

(3)



$$\overset{10}{\mathrm{H_3C}}\text{-}\underset{9}{\overset{\mathrm{OH}}{\mathrm{CH}}}\text{-}\overset{8}{\mathrm{SiH_2}}\text{-}\overset{7}{\mathrm{CH_2}}\text{-}\overset{6}{\mathrm{SiH_2}}\text{-}\overset{5}{\mathrm{CH_2}}\text{-}\overset{4}{\mathrm{SiH_2}}\text{-}\overset{3}{\mathrm{CH_2}}\text{-}\overset{2}{\mathrm{SiH_2}}\text{-}\overset{1}{\mathrm{CH_2}}\text{-OH}$$

2,4,6,8-tetrasiladecane-1,9-diol (PIN)
is senior to

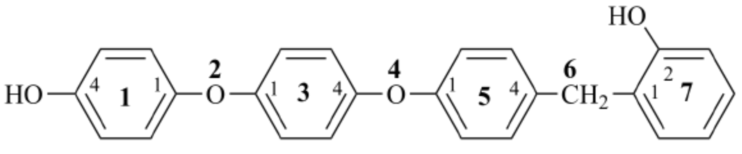


$$\text{HO-}\overset{10}{\mathrm{CH_2}}\text{-}\overset{9}{\mathrm{CH_2}}\text{-}\overset{8}{\mathrm{SiH_2}}\text{-}\overset{7}{\mathrm{CH_2}}\text{-}\overset{6}{\mathrm{SiH_2}}\text{-}\overset{5}{\mathrm{CH_2}}\text{-}\overset{4}{\mathrm{SiH_2}}\text{-}\overset{3}{\mathrm{CH_2}}\text{-}\overset{2}{\mathrm{SiH_2}}\text{-}\overset{1}{\mathrm{CH_2}}\text{-OH}$$

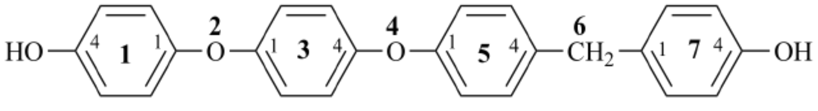
2,4,6,8-tetrasiladecane-1,10-diol (PIN)

[the locant set for the principal characteristic group ‘1,9’ is lower than ‘1,10’]

(4)



2,4-dioxa-1,7(1),3,5(1,4)-tetrabenzenaheptaphane-1^4,7^2-diol (PIN)
is senior to

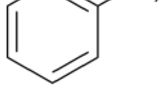


2,4-dioxa-1,7(1),3,5(1,4)-tetrabenzenaheptaphane-1^4,7^4-diol (PIN)

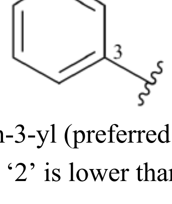
[the locant for the principal characteristic group ‘7^2’ is lower than ‘7^4’]

P-44.4.1.9 The senior ring or ring system has the lowest locants for points of attachment (if a substituent group) [criterion (i) in P-44.4.1].

Example (the symbol > means ‘is senior to’):



>



pyridin-2-yl (preferred prefix) pyridin-3-yl (preferred prefix)

[the locant for the point of attachment ‘2’ is lower than ‘3’]

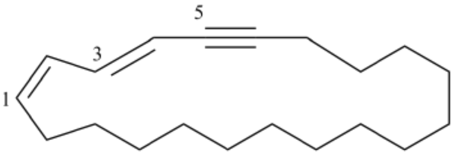
P-44.4.1.10 The senior ring, ring system or principal chain has the lowest locants for endings or prefixes that express changes in the degree of hydrogenation, i.e., for ‘ene’ and ‘yne’ endings and ‘hydro/dehydro’ prefixes [criterion (j) in P-44.4.1].

The prefixes hydro or dehydro are introduced in names by an additive or subtractive operation; thus, they are not included in the category of alphabetizable detachable prefixes describing substitution (P-15.1.3). In names, they occupy a place between nondetachable prefixes and the alphabetizable detachable prefixes. The prefixes hydro or dehydro express modifications of the degree of hydrogenation of a ring or ring system having the maximum number of noncumulative double bonds (a mancude structure) and are treated for numbering like the endings 'ene' and 'yne', which fulfill the same function. In names, the prefix 'dehydro' precedes the prefix 'hydro', when both are present. Simple numerical terms, such as 'di-','tetra-', etc., are used with 'hydro' and 'dehydro'.

P-44.4.1.10.1 For the endings 'ene' and 'yne' lower locants are assigned first to the endings as a set without regard to type and then to 'ene' endings.

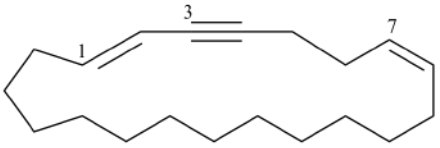
Example (the symbol > means 'is senior to'):

(1)



(1*Z*,3*E*)-cycloicosa-1,3-dien-5-yne (PIN)

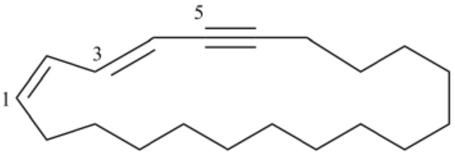
>



(1*E*)-cycloicosa-1,7-dien-3-yne (PIN)

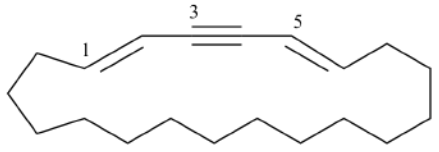
[the locant set '1,3,5' for the 'ene' and 'yne' endings is lower than '1,3,7']

(2)



(1*Z*,3*E*)-cycloicosa-1,3-dien-5-yne (PIN)

>



(1*E*,5*E*)-cycloicosa-1,5-dien-3-yne (PIN)

[the locant set '1,3' for the 'ene' endings is lower than '1,5']

(3)

11 10 9 8 7 6 5 4 3 2 1
$CH_3\text{-}CH_2\text{-}CH_2\text{-}C{\equiv}C\text{-}CH_2\text{-}CH{=}CH\text{-}CH{=}CH\text{-}CH_3$

undeca-2,4-dien-7-yne (PIN)
is senior to

11 10 9 8 7 6 5 4 3 2 1
$CH_3\text{-}CH_2\text{-}C{\equiv}C\text{-}CH_2\text{-}CH_2\text{-}CH{=}CH\text{-}CH{=}CH\text{-}CH_3$

undeca-2,4-dien-8-yne (PIN)

[the locant set '2,4,7' for the 'ene' and 'yne' endings is lower than '2,4,8']

(4)

1 2 3 4 5 6
$H_2C{=}CH\text{-}CH_2\text{-}CH{=}CH\text{-}CH_3$

hexa-1,4-diene (PIN)
is senior to

1 2 3 4 5 6
$H_2C{=}CH\text{-}CH_2\text{-}CH_2\text{-}CH{=}CH_2$

hexa-1,5-diene (PIN)

[the locant set '1,4' for the 'ene' endings is lower than '1,5']

(5)

11 10 9 8 7 6 5 4 3 2 1
$HO\text{-}CH_2\text{-}C{\equiv}C\text{-}CH{=}CH\text{-}CH_2\text{-}CH{=}CH\text{-}CH{=}CH\text{-}CH_2OH$

undeca-2,4,7-trien-9-yne-1,11-diol (PIN)
is senior to

11 10 9 8 7 6 5 4 3 2 1
$HO\text{-}CH_2\text{-}CH{=}CH\text{-}C{\equiv}C\text{-}CH_2\text{-}CH{=}CH\text{-}CH{=}CH\text{-}CH_2OH$

undeca-2,4,9-trien-7-yne-1,11-diol (PIN)

[the locant set '2,4,7' for the 'ene' endings is lower than '2,4,9']

(6)

1 3 6 10 13 14 16
$CH_3\text{-}CH_2\text{-}S\text{-}CH_2\text{-}CH_2\text{-}S\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}S\text{-}CH_2\text{-}CH_2\text{-}S\text{-}CH{=}CH\text{-}CH_3$

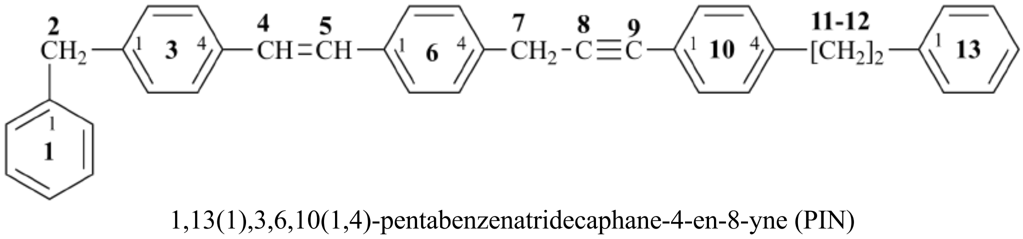
3,6,10,13-tetrathiahexadec-14-ene (PIN)
is senior to

1 3 6 10 13 15 16
$CH_3\text{-}CH_2\text{-}S\text{-}CH_2\text{-}CH_2\text{-}S\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}S\text{-}CH_2\text{-}CH_2\text{-}S\text{-}CH_2\text{-}CH{=}CH_2$

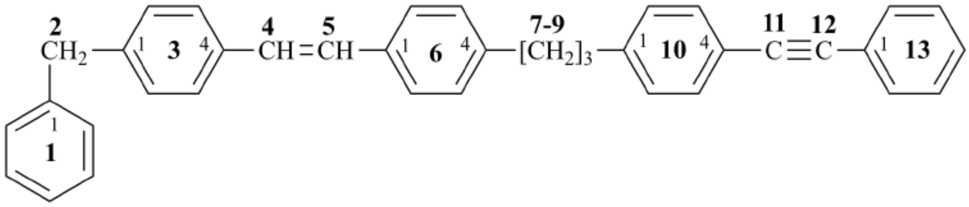
3,6,10,13-tetrathiahexadec-15-ene (PIN)

[the locant '14' for the 'ene' ending is lower than '15']

(7)

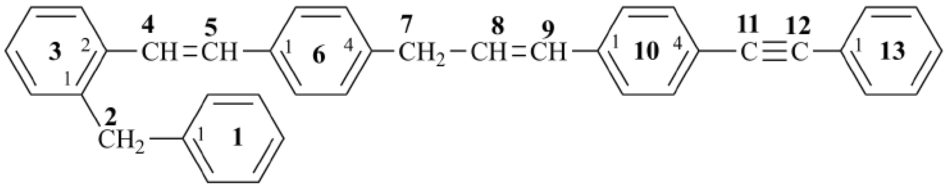


1,13(1),3,6,10(1,4)-pentabenzenatridecaphane-4-en-8-yne (PIN)
is senior to

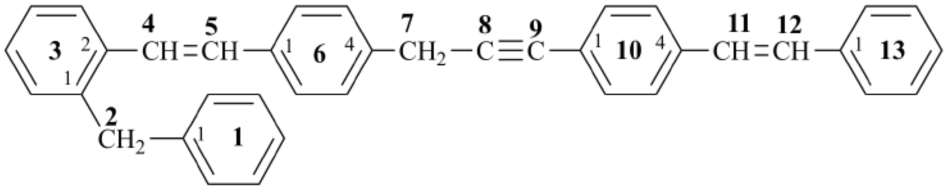

2
CH2
1
3
4
4
5
CH=CH
1
6
4
7-9
[CH2]3
1
10
4
11
12
C≡C
1
13
1
1

1,13(1),3,6,10(1,4)-pentabenzenatridecaphan-4-en-11-yne (PIN)
[the locant set ‘4,8’ for the ‘ene’ and ‘yne’ endings is lower than ‘4,11’]

(8)


3
2
1
4
5
CH=CH
1
6
4
7
8
9
CH2−CH=CH
1
10
4
11
12
C≡C
1
13
2
CH2
1
1

1,13(1),3(1,2),6,10(1,4)-pentabenzenatridecaphan-4,8-dien-11-yne (PIN)
is senior to

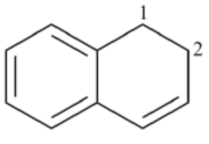

3
2
1
4
5
CH=CH
1
6
4
7
8
9
CH2−C≡C
1
10
4
11
12
CH=CH
1
13
2
CH2
1
1

1,13(1),3(1,2),6,10(1,4)-pentabenzenatridecaphane-4,11-dien-8-yne (PIN)
[the locant set ‘4,8’ for the ‘ene’ endings is lower than ‘4,11’]

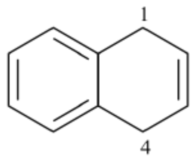
P-44.4.1.10.2 For ‘hydro/dehydro’ prefixes, lower locants are assigned as described in P-31.2.

Example (the symbol > means ‘is senior to’):

(1)

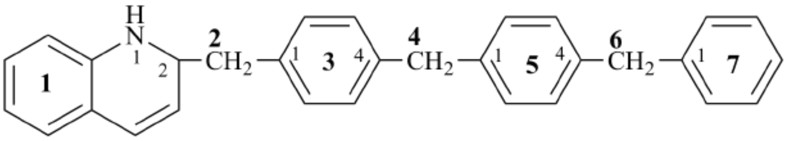


>

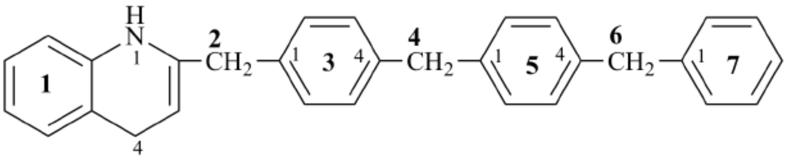


1,2-dihydronaphthalene (PIN) 1,4-dihydronaphthalene (PIN)
[the locant set for the ‘hydro’ prefixes ‘1,2’ is lower than ‘1,4’]

(2)

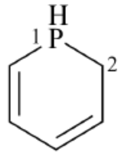

H
N
1
2
1
2
CH2
1
3
4
4
CH2
1
5
4
6
CH2
1
7

1^1,1^2-dihydro-1(2)-quinolina-3,5(1,4),7(1)-tribenzenaheptaphane (PIN)
is senior to

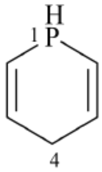

H
N
1
1
4
2
CH2
1
3
4
4
CH2
1
5
4
6
CH2
1
7

1^1,1^4-dihydro-1(2)-quinolina-3,5(1,4),7(1)-tribenzenaheptaphane (PIN)
[the locant set ‘1^1,1^2’ for the ‘hydro’ prefixes is lower than ‘1^1,1^4’]

(3)

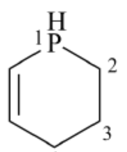


>

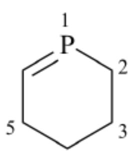


1,2-dihydrophosphinine (PIN) 1,4-dihydrophosphinine (PIN)
[the locant set ‘1,2’ for the ‘hydro’ prefixes is lower than ‘1,4’]

(4)



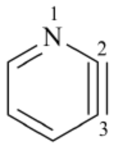
>



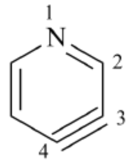
1,2,3,4-tetrahydrophosphinine (PIN) 2,3,4,5-tetrahydrophosphinine (PIN)

[the locant set ‘1,2,3,4’ for the ‘hydro’ prefixes is lower than ‘2,3,4,5’]

(5)



>



2,3-didehydropyridine (PIN) 3,4-didehydropyridine (PIN)

[the locant set ‘2,3’ for the ‘dehydro’ prefixes is lower than ‘3,4’]

Criteria for choosing a preferred IUPAC name based on a senior parent structure as described in P-44 are found in P-45.

P-44.4.1.11 The senior ring, ring system, or principal chain that has one or more isotopically modified atoms [criterion (k) in P-44.4.1].

When there is a choice for the senior parent structure between isotopically modified and isotopically unmodified compounds or between isotopically modified compounds (see Chapter P-8), the senior parent structure is chosen according to the following criteria, applied successively until a decision can be made. In structures and names, nuclide symbols enclosed in parentheses describe isotopic substitution; nuclide symbols enclosed in square brackets describe isotopic labeling (see Chapter P-8).

P-44.4.1.11.1 The senior parent structure contains the greater number of isotopically modified atoms or groups.

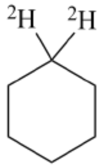
Example (the symbol > means ‘is senior to’):

5 4 3 2 1 5 4 3 2 1

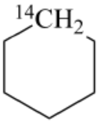
CH_3-CH_2-CH_2-CH_2-$CH_2{}^{2}H$ > CH_3-CH_2-CH_2-CH_2-CH_3

(1-$^{2}H_1$)pentane (PIN) pentane (PIN)

[one isotopically modified atom is senior to none]



>

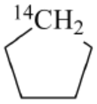


(1,1-$^{2}H_2$)cyclohexane (PIN) ($^{14}C_1$)cyclohexane (PIN)

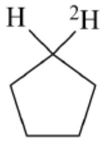
[two ^{2}H atoms are senior to one ^{14}C]

P-44.4.1.11.2 The senior parent structure has the greater number of nuclides of higher atomic number for modified atoms or groups.

Example (the symbol > means ‘is senior to’):



>



($^{14}C_1$)cyclopentane (PIN) ($^{2}H_1$)cyclopentane (PIN)

[^{14}C is senior to ^{2}H]

5 4 3 2 1 5 4 3 2 1

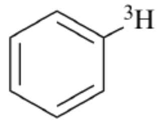
CH_3-CH_2-CH_2-CH_2-[^{14}C]H_3 > CH_3-CH_2-CH_2-CH_2-CH_2[^{2}H]

[1-^{14}C]pentane (PIN) [1-$^{2}H_1$]pentane (PIN)

[^{14}C is senior to ^{2}H]

P-44.4.1.11.3 The senior parent structure has the greater number of nuclides of higher mass number for modified atoms or groups.

Example (the symbol > means ‘is senior to’):



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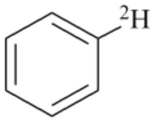


($^{3}H_1$)benzene (PIN) ($^{2}H_1$)benzene (PIN)

[^{3}H is senior to ^{2}H]

$\overset{5}{C}H_3\text{-}\overset{4}{C}H_2\text{-}\overset{3}{C}H_2\text{-}\overset{2}{C}H_2\text{-}[^{14}\overset{1}{C}]H_3$ > $\overset{5}{C}H_3\text{-}\overset{4}{C}H_2\text{-}\overset{3}{C}H_2\text{-}\overset{2}{C}H_2\text{-}[^{13}\overset{1}{C}]H_3$

[1-^{14}C]pentane (PIN) [1-^{13}C]pentane (PIN)

[^{14}C is senior to ^{13}C]

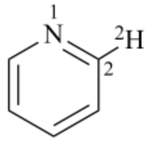
P-44.4.1.11.4 The senior parent structure has the lowest locant(s) for isotopically modified atoms or groups.

Example (the symbol > means ‘is senior to’):

$HOO\overset{1}{C}\text{-}\overset{2}{C}H_2\text{-}\overset{3}{C}H_2\text{-}\overset{4}{C}H[^2H]\text{-}\overset{5}{C}H_3$ > $HOO\overset{1}{C}\text{-}\overset{2}{C}H_2\text{-}\overset{3}{C}H_2\text{-}\overset{4}{C}H_2\text{-}\overset{5}{C}H_2[^2H]$

[4-^{2}H$_1$]pentanoic acid (PIN) [5-^{2}H$_1$]pentanoic acid (PIN)

[4-^{2}H is senior to 5-^{2}H]



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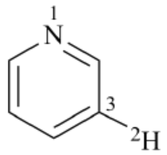


(2-^{2}H)pyridine (PIN) (3-^{2}H)pyridine (PIN)

[2-^{2}H is senior to 3-^{2}H]

P-44.4.1.11.5 The senior parent structure has the lower locant(s) for nuclides of higher atomic number for modified atoms or groups;

Example (the symbol > means ‘is senior to’):

$HOO\overset{1}{C}\text{-}\overset{2}{C}H_2\text{-}\overset{3}{C}H_2\text{-}[^{13}\overset{4}{C}]H_2\text{-}\overset{5}{C}H_2[^2H]$ > $HOO\overset{1}{C}\text{-}\overset{2}{C}H_2\text{-}\overset{3}{C}H_2\text{-}\overset{4}{C}H[^2H]\text{-}[^{13}\overset{5}{C}]H_3$

[4-^{13}C,5-^{2}H$_1$]pentanoic acid (PIN) [5-^{13}C,4-^{2}H$_1$]pentanoic acid (PIN)

[4-^{13}C is senior to 5-^{13}C]

P-44.4.1.11.6 The senior parent structure has the lowest locant(s) for nuclides of higher mass number for modified atoms or groups.

Example (the symbol > means ‘is senior to’):

$HO\overset{1}{C}H_2\text{-}\overset{2}{C}H_2\text{-}[^{14}\overset{3}{C}]H_2\text{-}[^{13}\overset{4}{C}]H_3$ > $HO\overset{1}{C}H_2\text{-}\overset{2}{C}H_2\text{-}[^{13}\overset{3}{C}]H_2\text{-}[^{14}\overset{4}{C}]H_3$

[4-^{13}C,3-^{14}C]butan-1-ol (PIN) [3-^{13}C,4-^{14}C]butan-1-ol (PIN)

[3-^{14}C is senior to 4-^{14}C]

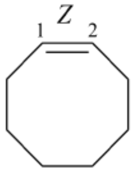
P-44.4.1.12 The senior ring, ring system, or principal chain has one or more stereogenic centers [criterion (l) in P-44.4.1].

P-44.4.1.12.1 ‘*cis/trans*’ Isomerism, the ‘*E/Z*’ convention

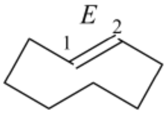
When there is a choice between parent structures that differ only by ‘*Z*’ and ‘*E*’ configurations, the senior parent structure contains the greater number of double bonds with ‘*Z*’ configuration; when a further choice is required, the senior parent structure has the lowest locant set for the double bond(s) with the ‘*Z*’ configuration. For the meaning of ‘*Z*’ and ‘*E*’ see Chapter P-9.

Example (the symbol > means ‘is senior to’):

(1)



>

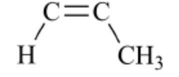


(*Z*)-cyclooctene (PIN)
cis-cyclooctene

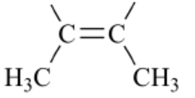
(*E*)-cyclooctene (PIN)
trans-cyclooctene

[‘*Z*’ is senior to ‘*E*’]

(2)



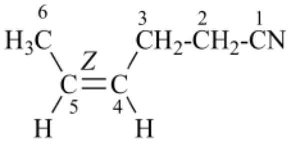
>



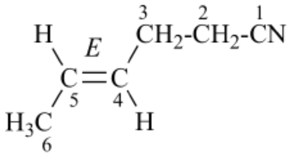
(2*Z*)-2-methylbut-2-enoic acid (PIN) (2*E*)-2-methylbut-2-enoic acid (PIN)

[‘*Z*’ is senior to ‘*E*’]

(3)


6
H₃C
3 2 1
CH₂-CH₂-CN
Z
C=C
5 4
H H

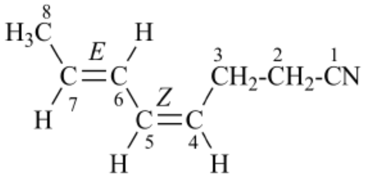
>


3 2 1
H
E
CH₂-CH₂-CN
C=C
5 4
H₃C
6
H

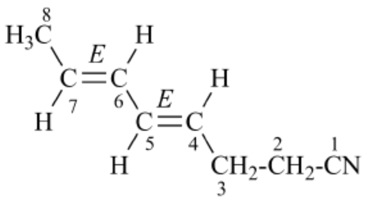
(4*Z*)-hex-4-enenitrile (PIN) (4*E*)-hex-4-enenitrile (PIN)

[‘*Z*’ is senior to ‘*E*’]

(4)

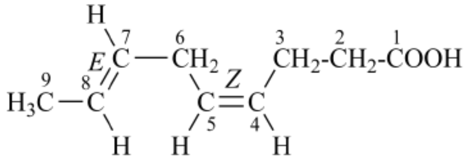

8
H₃C
H
E
3 2 1
C=C
CH₂-CH₂-CN
7 6
Z
H
C=C
5 4
H H

(4*Z*,6*E*)-octa-4,6-dienoic acid (PIN)
is senior to

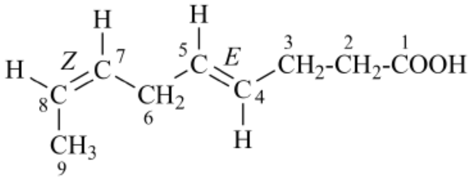

8
H₃C
H
E
C=C
H
7 6
E
H
C=C
5 4
H
2 1
CH₂-CH₂-CN
3

(4*E*,6*E*)-octa-4,6-dienoic acid (PIN)
[‘*Z*,*E*’ is senior to ‘*E*,*E*’]

(5)


H
7 6
E C—CH₂
3 2 1
CH₂-CH₂-COOH
9 8
Z
H₃C—C
C=C
5 4
H H H

(4*Z*,7*E*)-nona-4,7-dienoic acid (PIN)
is senior to


H
H
Z C 7
5 C E
3 2 1
CH₂-CH₂-COOH
H
C
8
CH₂
6
C 4
CH₃
9
H

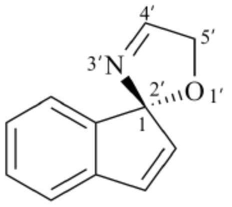
(4*E*,7*Z*)-nona-4,7-dienoic acid (PIN)
[‘4*Z*,7*E*’ is senior to ‘4*E*,7*Z*’]

P-44.4.1.12.2 Enantiomerism, the ‘*R*’ and ‘*S*’ stereodescriptors

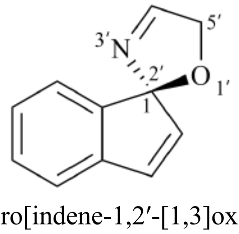
When there is a choice between parent structures differing only by the configurations of the chirality centers, the principal chain or the senior ring system is chosen by applying the CIP sequence rules 4 and 5, in the order: *like* stereodescriptors such as ‘*RR*’, ‘*SS*’ have priority over *unlike* ‘*RS*’ and ‘*SR*’ (‘*l*’ has priority over ‘*u*’), the ‘*r*’ over ‘*s*’, then ‘*R*’ over ‘*S*’. The CIP Sequence Rules are described in Chapter P-9.

Example (the symbol > means ‘is senior to’):

(1)



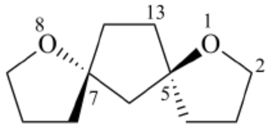
(1*R*)-5′*H*-spiro[indene-1,2′-[1,3]oxazole] (PIN)
is senior to



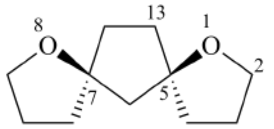
(1*S*)-5′*H*-spiro[indene-1,2′-[1,3]oxazole] (PIN)

[‘*R*’ is senior to ‘*S*’]

(2)



(5*R*,7*R*)-1,8-dioxadispiro[4.1.4^7.2^5]tridecane (PIN)
is senior to

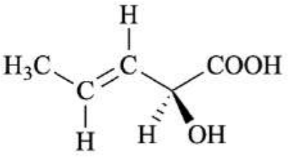


(5*R*,7*S*)-1,8-dioxadispiro[4.1.4^7.2^5]tridecane (PIN)
[‘*RR*’ is senior to ‘*RS*’]

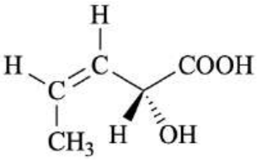
P-44.4.1.12.3 ‘*cis/trans*’ Isomerism (the ‘*E/Z*’ convention) and enantiomerism (the ‘*R/S*’ convention)

When there is a choice between parent structures that contain both ‘*E/Z*’ (or *cis/trans*) and ‘*R/S*’ descriptors the ‘*E/Z*’ (or *cis/trans*) descriptors are preferred to the ‘*R/S*’ descriptors.

Example



>



(2*R*,3*Z*)-2-hydroxypent-3-enoic acid (2*S*,3*E*)-2-hydroxypent-3-enoic acid
[*Z* is senior to *E*]

P-45 SELECTION OF PREFERRED IUPAC NAMES

P-45.0 INTRODUCTION

Two or more names may result based on the same senior parent structure selected according to P-44, because of different substitution patterns or multiple occurrences of the same senior parent structure. A parent structure is defined (P-15.1) as a parent hydride, for example, benzene, a functionalized parent hydride, for example cyclohexanol, or a functional parent compound, for example, acetic acid. Application of the criteria in this section will generate the preferred IUPAC name.

P-45.1 Multiplication of identical senior parent structures
P-45.2 Criteria related to number and location of substituent groups
P-45.3 Criteria related only to substituents with nonstandard bonding numbers, other criteria being equal
P-45.4 Criteria related only to isotopic modification of substituents
P-45.5 Criteria related to alphanumerical order of names
P-45.6 Criteria related only to configuration

P-45.1 MULTIPLICATION OF IDENTICAL SENIOR PARENT STRUCTURES

P-45.1.1 Multiplicative nomenclature is senior to substitutive nomenclature for generating preferred IUPAC names to express multiple occurrences of identical senior parent structures, other than alkanes, in the name of the parent structure (see P-51.3.1). In most cases multiplicative names are shorter than regular substitutive names. A preferred IUPAC name is generated by multiplicative nomenclature when the following criteria for its use are met (see P-51.3.1).

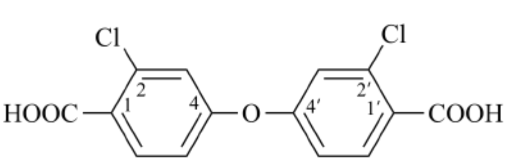
(1) the linking bonds (single or multiple) between the central substituent group of the multiplicative group and all subsequent structural units are identical; and

(2) the multiplicative groups, other than the central multiplicative group, are symmetrically substituted; and

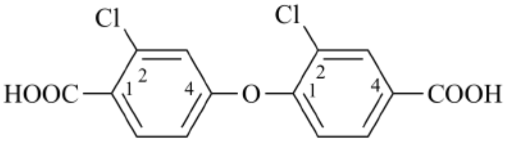
(3) the locants of all substituent groups on the identical parent structures, including suffix groups, are identical.

When these conditions are not met, substitutive nomenclature generates preferred IUPAC names.

Example:



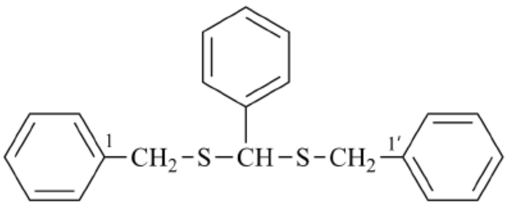
4,4′-oxybis(2-chlorobenzoic acid) (PIN, multiplicative name) but



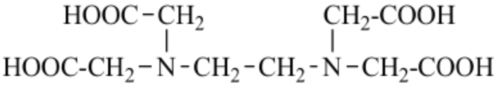
4-(4-carboxy-2-chlorophenoxy)-2-chlorobenzoic acid (PIN, substitutive name)

P-45.1.2 When two or more parent structures, rings, ring systems, or chains, satisfy the requirements for multiplicative nomenclature (see P-15.3), the structure chosen as the parent structure to be multiplied is the more numerous.

Examples:

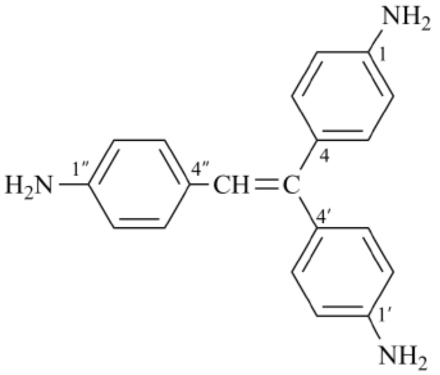


1,1′-[(phenylmethylene)bis(sulfanediylmethylene)]dibenzene (PIN)
(multiplication of three benzene rings is not possible)

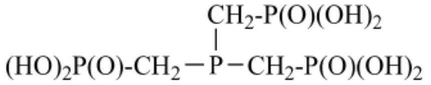


$$\begin{array}{ccccc} & \mathrm{HOOC{-}CH_2} & & \mathrm{CH_2{-}COOH} & \\ & | & & | & \\ \mathrm{HOOC{-}CH_2{-}} & \mathrm{N} & \mathrm{{-}CH_2{-}CH_2{-}} & \mathrm{N} & \mathrm{{-}CH_2{-}COOH} \end{array}$$

2,2′,2″,2‴-(ethane-1,2-diyldinitrilo)tetraacetic acid
N,*N*′-(ethane-1,2-diyl)bis[*N*-(carboxymethyl)glycine]

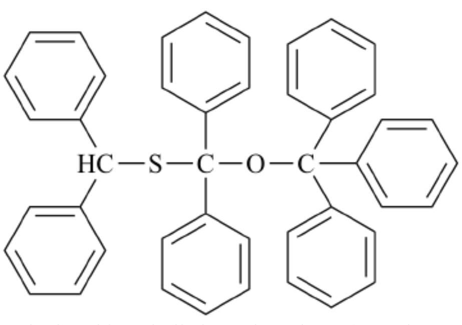


4,4′,4″-(ethene-1,1,2-triyl)trianiline (PIN)
[not 4,4′-[2-(4-aminophenyl)ethene-1,1-diyl]dianiline;
the PIN multiplies three parent structures;
the second name multiplies only two]



$$\begin{array}{ccc} & \mathrm{CH_2\text{-}P(O)(OH)_2} & \\ & | & \\ \mathrm{(HO)_2P(O)\text{-}CH_2{-}} & \mathrm{P} & \mathrm{{-}CH_2\text{-}P(O)(OH)_2} \end{array}$$

[phosphanetriyltris(methylene)]tris(phosphonic acid) (PIN)



1,1′,1″-({[(diphenylmethyl)sulfanyl]diphenylmethoxy}methanetriyl)tribenzene (PIN)
(not 1,1′-({[diphenyl(triphenylmethoxy)methyl]sulfanyl}methylene)dibenzene;
the PIN multiplies three parent structures;
the second name multiplies only two)

P-45.2 CRITERIA RELATED TO NUMBER AND LOCATION OF SUBSTITUENT GROUPS

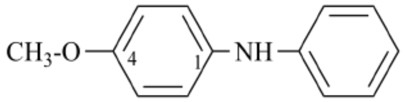
The following criteria are applied, in turn, until a decision is reached. The preferred IUPAC name is the name based on the senior parent structure that has:

P-45.2.1 the maximum number of substituent groups cited as prefixes;
P-45.2.2 the lower locant set for substituent groups cited as prefixes;
P-45.2.3 the lower locant set for substituent groups in order of citation in the name

P-45.2.1 The preferred IUPAC name is based on the senior parent structure that has the maximum number of substituents cited as prefixes (other than ‘hydro/dehydro’) to the parent structure.

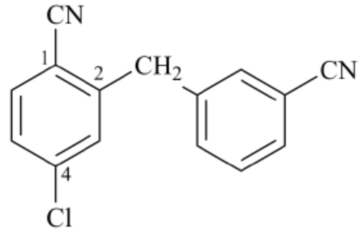
Examples:

(1)



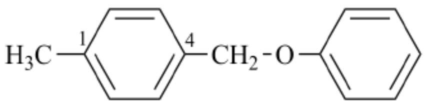
4-methoxy-*N*-phenylaniline (PIN)
[not *N*-(4-methoxyphenyl)aniline;
the PIN parent structure has more substituents,
two simple substituents *vs.* one compound substituent]

(2)



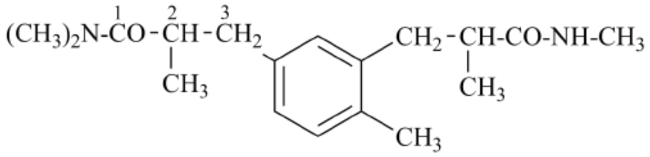
4-chloro-2-[(3-cyanophenyl)methyl]benzonitrile (PIN)
[not 3-[(5-chloro-2-cyanophenyl)methyl]benzonitrile;
the PIN parent structure has more substituents,
two (one simple and one complex) substituents *vs.* one complex substituent]

(3)



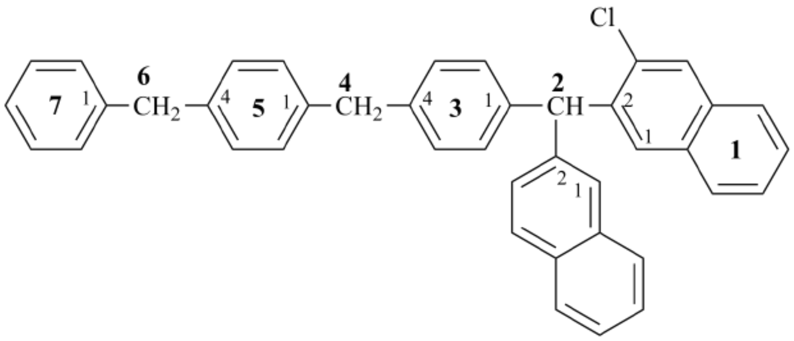
1-methyl-4-(phenoxymethyl)benzene (PIN)
[not [(4-methylphenyl)methoxy]benzene;
the PIN parent structure has more substituents;
two (one simple and one compound) substituent *vs.* one complex substituent]

(4)



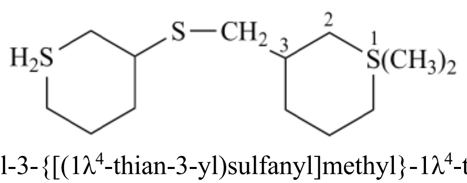
N,*N*,2-trimethyl-3-{4-methyl-3-[2-methyl-3-(methylamino)-3-oxopropyl]phenyl}propanamide (PIN)
[not 3-{5-[(3-dimethylamino)-2-methyl-3-oxopropyl]-2-methylphenyl}-*N*,2-dimethylpropanamide;
the PIN parent structure has more substituents,
four (three simple and one complex) substituents *vs.* three (two simple and one complex)]

(5)



1^3-chloro-2-(naphthalen-2-yl)-1(2)-naphthalena-3,5(1,4),7(1)-tribenzenaheptaphane (PIN)
[not 2-(3-chloronaphthalen-2-yl)-1(2)-naphthalena-3,5(1,4),7(1)-tribenzenaheptaphane;
the PIN parent structure has more substituents, two simple substituents *vs.* one compound substituent]

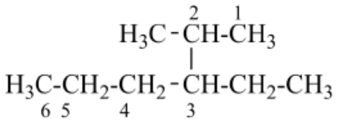
(6)



1,1-dimethyl-3-{[($1\lambda^4$-thian-3-yl)sulfanyl]methyl}-$1\lambda^4$-thiane (PIN)
[not 3-{[(1,1-dimethyl-$1\lambda^4$-thian-3-yl)methyl]sulfanyl}-$1\lambda^4$-thiane;
the PIN parent structure has more substituents,

three (two simple and one complex) substituents *vs.* one complex substituent]

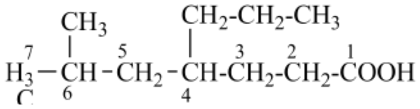
(7)



$$\begin{array}{l} \qquad\qquad\quad H_3C\text{-}\overset{2}{C}H\text{-}\overset{1}{C}H_3 \\ \qquad\qquad\qquad\quad | \\ H_3\underset{6}{C}\text{-}\underset{5}{C}H_2\text{-}\underset{4}{C}H_2\text{-}\underset{3}{C}H\text{-}CH_2\text{-}CH_3 \end{array}$$

3-ethyl-2-methylhexane (PIN)
[not 3-isopropylhexane or 3-(propan-2-yl)hexane;
the PIN parent structure has more substituents,
two simple substituents *vs.* one simple substituent)

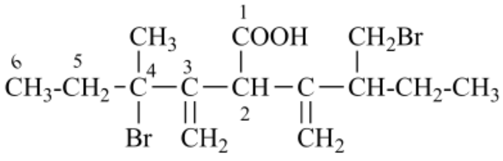
(8)



$$\begin{array}{l} \quad CH_3 \qquad\qquad CH_2\text{-}CH_2\text{-}CH_3 \\ \quad\ | \qquad\qquad\quad\ \ | \\ H_3\overset{7}{C}-\underset{6}{C}H\text{-}\overset{5}{C}H_2\text{-}\underset{4}{C}H\text{-}\overset{3}{C}H_2\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}OOH \end{array}$$

6-methyl-4-propylheptanoic acid (PIN)
[not 4-(2-methylpropyl)heptanoic acid;
the principal chain has more substituent,
two simple substituents *vs.* one compound substituent]

(9)



$$\begin{array}{l} \qquad\qquad\quad CH_3 \qquad \overset{1}{C}OOH \quad CH_2Br \\ \qquad\qquad\quad\ | \qquad\qquad | \qquad\quad\ | \\ \overset{6}{C}H_3\text{-}\overset{5}{C}H_2\text{-}\overset{4}{C}-\overset{3}{C}-\underset{2}{C}H-C-CH\text{-}CH_2\text{-}CH_3 \\ \qquad\qquad\quad\ | \quad\ \ \| \qquad\qquad \| \\ \qquad\qquad\ Br \ \ CH_2 \qquad\quad CH_2 \end{array}$$

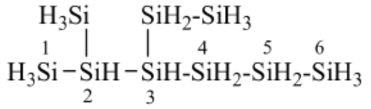
4-bromo-2-[3-(bromomethyl)pent-1-en-2-yl]-4-methyl-3-methylidenehexanoic acid (PIN)
[not 4-(bromomethyl)-2-(3-bromo-3-methylpent-1-en-2-yl)-3-methylidenehexanoic acid;
the PIN parent chain has more substituents;
four (three simple and one complex) substituents *vs.* three (one simple and two compound)]

(10)

$$(CH_3)_3\overset{1}{Si}\text{-}\overset{2}{Si}H_2\text{-}S\text{-}S\text{-}SiH_2\text{-}SiH_3$$

2-(disilanyldisulfanyl)-1,1,1-trimethyldisilane (PIN)
[not [2-(2,2,2-trimethyldisilanyl)disulfan-1-yl]disilane;
the PIN parent structure has more substituents,
four (three simple and one compound) substituents *vs.* one complex substituent]

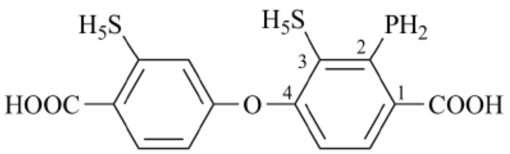
(11)



$$\begin{array}{l} \quad H_3Si \qquad SiH_2\text{-}SiH_3 \\ \qquad\ \ | \qquad\quad | \\ H_3\overset{1}{Si}-\underset{2}{Si}H-\underset{3}{Si}H\text{-}\overset{4}{Si}H_2\text{-}\overset{5}{Si}H_2\text{-}\overset{6}{Si}H_3 \end{array}$$

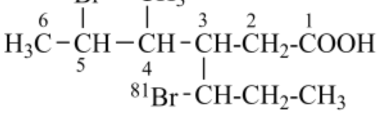
3-disilanyl-2-silylhexasilane (preselected name, see P-12.2)
[not 3-(trisilan-2-yl)hexasilane or 3-(1-silyldisilanyl)hexasilane;
the PIN parent chain has more substituents, two simple substituents *vs.* one simple or one compound substituent]

(12)



4-[4-carboxy-3-(λ^6-sulfanyl)phenoxy]-2-phosphanyl-3-(λ^6-sulfanyl)benzoic acid (PIN)
[not 4-[4-carboxy-3-phosphanyl-2-(λ^6-sulfanyl)phenoxy]-2-(λ^6-sulfanyl)benzoic acid)
the PIN parent structure has more substituents,
three (two simple and one compound) substituents *vs.* two (one simple and one complex)]

(13)



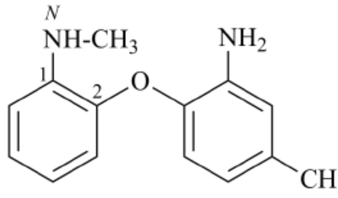
$$\begin{array}{l} \qquad\ \ {}^{81}Br \quad CH_3 \\ \qquad\quad | \qquad\ | \\ H_3C-\overset{6}{\underset{5}{C}}H-\underset{4}{C}H\text{-}\overset{3}{C}H\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}OOH \\ \qquad\qquad\qquad\quad | \\ \qquad\qquad\quad {}^{81}Br\text{-}CH\text{-}CH_2\text{-}CH_3 \end{array}$$

5-(^{81}Br)bromo-3-[1-(^{81}Br)bromopropyl]-4-methylhexanoic acid (PIN)
[not 4-(^{81}Br)bromo-3-[3-(^{81}Br)bromobutan-2-yl]hexanoic acid;
the PIN parent chain has more substituents,
three (two simple and one compound) *vs.* two (one simple and one compound)]

P-45.2.2 The preferred IUPAC name is based on the senior parent structure that has the lower locant or set of locants for substituents cited as prefixes (other than 'hydro/dehydro') to the parent structure.

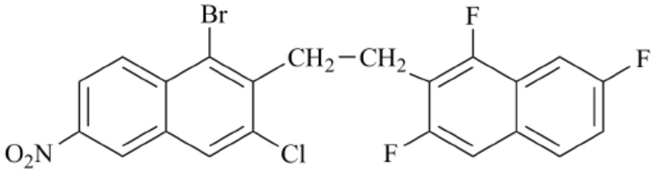
Examples:

(1)



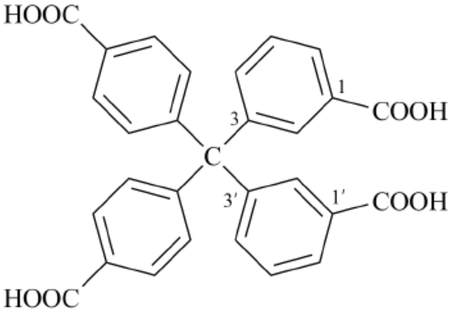
2-(2-amino-4-methylphenoxy)-*N*-methylaniline (PIN)
[not 5-methyl-2-[2-(methylamino)phenoxy]aniline;
the locant set ‘*N*,2’ in the PIN is lower than ‘2,5’]

(2)



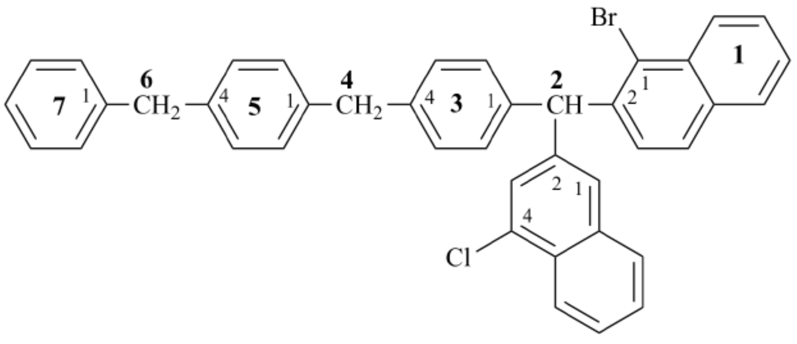
1-bromo-3-chloro-6-nitro-2-[2-(1,3,7-trifluoronaphthalen-2-yl)ethyl]naphthalene (PIN)
[not 2-[2-(1-bromo-3-chloro-6-nitronaphthalen-2-yl)ethyl]-1,3,7-trifluoronaphthalene;
the locant set ‘1,2,3,6’ in the PIN is lower than ‘1,2,3,7’]

(3)



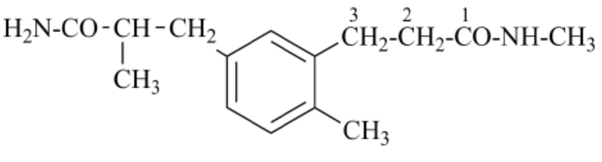
3,3′-[bis(4-carboxyphenyl)methylene]dibenzoic acid (PIN)
[not 4,4′-[bis(3-carboxyphenyl)methylene]dibenzoic acid;
the locant set 3,3′ in the PIN is lower than 4,4′]

(4)



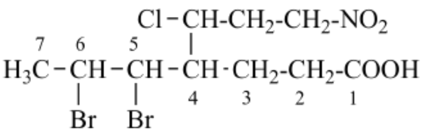
1^1-bromo-2-(4-chloronaphthalen-2-yl)-1(2)-naphthalena-3,5(1,4),7(1)-tribenzenaheptaphane (PIN)
[not 2-(1-bromonaphthalen-2-yl)-1^4-chloro-1(2)-naphthalena-3,5(1,4),7(1)-tribenzenaheptaphane;
the locant set ‘1^1,2’ in the PIN is lower than the locant set ‘1^4,2’]

(5)



3-[5-(3-amino-2-methyl-3-oxopropyl)-2-methylphenyl]-*N*-methylpropanamide (PIN)
[not 2-methyl-3-{4-methyl-3-[3-(methylamino)-3-oxopropyl]phenyl}propanamide;
the locant set ‘*N*,3’ in the PIN is lower than ‘2,3’]

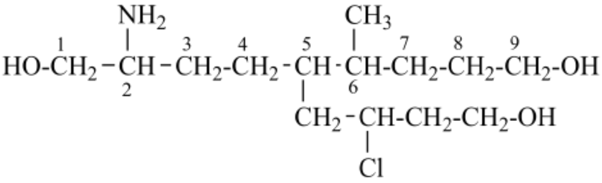
(6)



$$\mathrm{\overset{7}{H_3C}-\underset{\underset{Br}{|}}{\overset{6}{C}H}-\underset{\underset{Br}{|}}{\overset{5}{C}H}-\overset{Cl-CH-CH_2-CH_2-NO_2}{\overset{|}{\underset{4}{C}H}}-\underset{3}{CH_2}-\underset{2}{CH_2}-\underset{1}{COOH}}$$

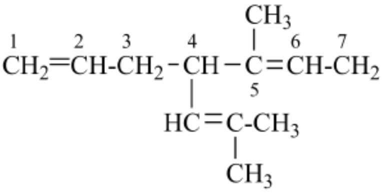
5,6-dibromo-4-(1-chloro-3-nitropropyl)heptanoic acid (PIN)
[not 5-chloro-4-(1,2-dibromopropyl)-7-nitroheptanoic acid;
the locant set ‘4,5,6’ in the PIN is lower than ‘4,5,7’]

(7)


NH2
CH3
HO-CH2-CH-CH2-CH2-CH-CH-CH2-CH2-CH2-OH
CH2-CH-CH2-CH2-OH
Cl
1
2
3
4
5
6
7
8
9

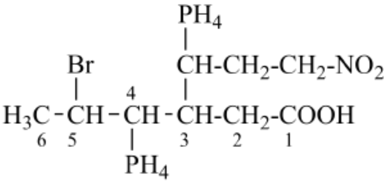
2-amino-5-(2-chloro-4-hydroxybutyl)-6-methylnonane-1,9-diol (PIN)
[not 2-amino-7-chloro-5-(5-hydroxypentan-2-yl)nonane-1,9-diol;
not 5-(3-amino-4-hydroxybutyl)-3-chloro-6-methylnonane-1,9-diol;
the locant set ‘2,5,6’ in the PIN is lower than the locant set ‘2,5,7’ or ‘3,5,6’]

(8)


CH3
CH2=CH-CH2-CH-C=CH-CH2
HC=C-CH3
CH3
1
2
3
4
5
6
7

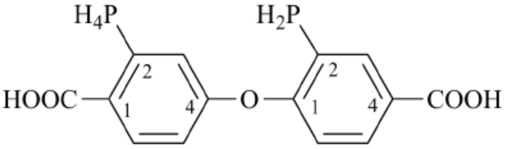
5-methyl-4-(2-methylprop-1-en-1-yl)hepta-1,5-diene (PIN)
[not 4-(but-2-en-2-yl)-6-methylhepta-1,5-diene;
the locant set ‘4,5’ in the PIN is lower than ‘4,6’]

(9)


PH4
Br
CH-CH2-CH2-NO2
H3C-CH-CH-CH-CH2-COOH
PH4
6
5
4
3
2
1

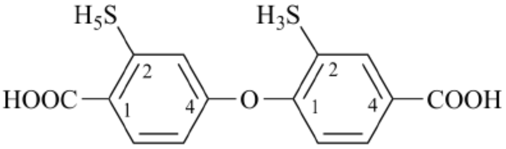
5-bromo-3-[3-nitro-1-(λ^5-phosphanyl)propyl]-4-(λ^5-phosphanyl)hexanoic acid (PIN)
[not 3-[2-bromo-1-(λ^5-phosphanyl)propyl]-6-nitro-4-(λ^5-phosphanyl)hexanoic acid,
the locant set ‘3,4,5’ in the PIN is lower than the locant set ‘3,4,6’]

(10)


H4P
H2P
HOOC
O
COOH
1
2
4
1
2
4

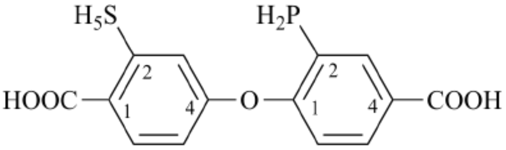
4-(4-carboxy-2-phosphanylphenoxy)-2-(λ^5-phosphanyl)benzoic acid (PIN)
[not 4-[4-carboxy-3-(λ^5-phosphanyl)phenoxy]-3-phosphanylbenzoic acid;
the locant set ‘2,4’ in the PIN is lower than ‘3,4’]

(11)


H5S
H3S
HOOC
O
COOH
1
2
4
1
2
4

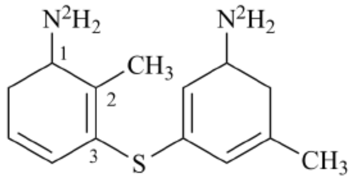
4-[4-carboxy-2-(λ^4-sulfanyl)phenoxy]-2-(λ^6-sulfanyl)benzoic acid (PIN)
[not 4-[4-carboxy-3-(λ^6-sulfanyl)phenoxy]-3-(λ^4-sulfanyl)benzoic acid;
the locant set ‘2,4’ in the PIN is lower than ‘3,4’]

(12)


H5S
H2P
HOOC
O
COOH
1
2
4
1
2
4

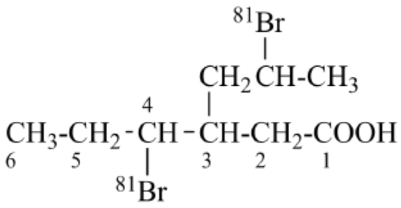
4-(4-carboxy-2-phosphanylphenoxy)-2-(λ^6-sulfanyl)benzoic acid (PIN)
[not 4-[4-carboxy-3-(λ^6-sulfanyl)phenoxy]-3-phosphanylbenzoic acid;
the locant set ‘2,4’ in the PIN is lower than ‘3,4’]

(13)


N2H2
N2H2
1
CH3
2
3
S
CH3

3-{[3-($^2H_2$)amino-5-methylcyclohexa-1,5-dien-1-yl]sulfanyl}-2-methylcyclohexa-2,4-dien-1-($^2H_2$)amine (PIN)
[not 3-{[3-($^2H_2$)amino-2-methylcyclohexa-1,5-dien-1-yl]sulfanyl}-5-methylcyclohexa-2,4-dien-1-($^2H_2$)amine,
the locant set ‘2,3’ in the PIN is lower than ‘3,5’]

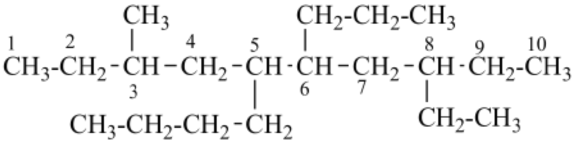
(14)



$$\mathrm{\underset{6}{CH_3}\text{-}\underset{5}{CH_2}\text{-}\underset{^{81}Br}{\overset{4}{CH}}\text{-}\underset{3}{\overset{CH_2CH(^{81}Br)\text{-}CH_3}{CH}}\text{-}\underset{2}{CH_2}\text{-}\underset{1}{COOH}}$$

4-(^{81}Br)bromo-3-[2-(^{81}Br)bromopropyl]hexanoic acid (PIN)
[not 5-(^{81}Br)bromo-3-[1-(^{81}Br)bromopropyl]hexanoic acid,
the locant set in the PIN, ‘3,4’ is lower than ‘3,5’]

(15)



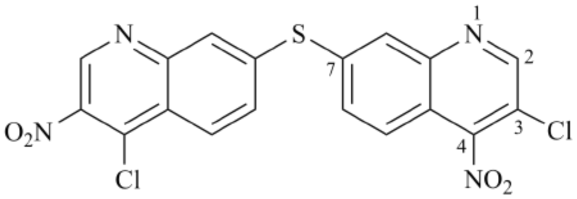
$$\mathrm{\overset{1}{CH_3}\text{-}\overset{2}{CH_2}\text{-}\underset{3}{\overset{CH_3}{CH}}\text{-}\overset{4}{CH_2}\text{-}\underset{CH_3\text{-}CH_2\text{-}CH_2\text{-}CH_2}{\overset{5}{CH}}\text{-}\underset{6}{\overset{CH_2\text{-}CH_2\text{-}CH_3}{CH}}\text{-}\underset{7}{CH_2}\text{-}\underset{CH_2\text{-}CH_3}{\overset{8}{CH}}\text{-}\overset{9}{CH_2}\text{-}\overset{10}{CH_3}}$$

3-chloro-5-(3-hydroxybutyl)-4,6-dimethylnonane-2,8-diol (PIN)
[not 7-chloro-5-(3-hydroxybutyl)-4,6-dimethylnonane-2,8-diol:
the locant set of the PIN is ‘3,4,5,6’ which is lower than ‘4,5,6,7’]

P-45.2.3 The preferred IUPAC name is based on the senior parent structure that has the lower locant or set of locants for substituents cited as prefixes to the parent structure (other than ‘hydro/dehydro’ prefixes) in their order of citation in the name.

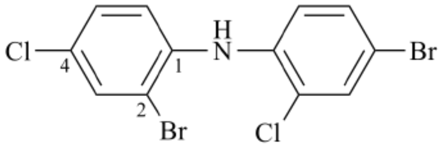
Examples:

(1)



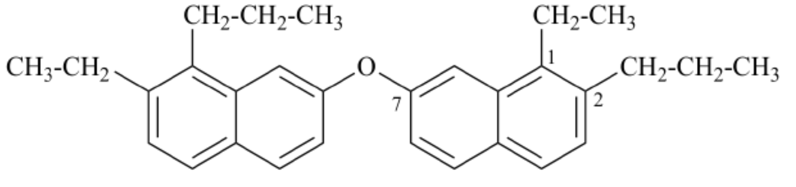
3-chloro-7-[(4-chloro-3-nitroquinolin-7-yl)sulfanyl]-4-nitroquinoline (PIN)
[not 4-chloro-7-[(3-chloro-4-nitroquinolin-7-yl)sulfanyl]-3-nitroquinoline,
the locant sets are the same in both names, i.e., ‘3,4,7’, but in their order
of appearance in the name the locant set ‘3,7,4’ in the PIN is lower than ‘4,7,3’]

(2)



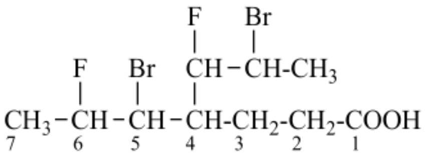
2-bromo-*N*-(4-bromo-2-chlorophenyl)-4-chloroaniline (PIN)
[not 4-bromo-*N*-(2-bromo-4-chlorophenyl)-2-chloroaniline;
the locant sets are the same, i.e., ‘*N*,2,4’, but in their order
of appearance in the name the locant set ‘2,*N*,4’ in the PIN is lower than ‘4,*N*,2’]

(3)



1-ethyl-7-[(7-ethyl-8-propylnaphthalen-2-yl)oxy]-2-propylnaphthalene (PIN)
[not 2-ethyl-7-[(8-ethyl-7-propylnaphthalen-2-yl)oxy]-1-propylnaphthalene,
the locant sets are the same in both names, i.e., ‘1,2,7’, but in their order
of appearance in the name, the locant set in the PIN ‘1,7,2’ is lower than ‘2,7,1’]

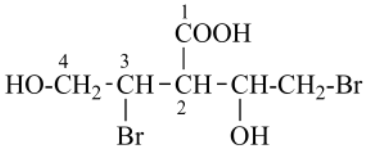
(4)



$$\mathrm{\underset{7}{CH_3}\text{-}\underset{6}{\overset{F}{CH}}\text{-}\underset{5}{\overset{Br}{CH}}\text{-}\underset{4}{\overset{\overset{F\quad Br}{CH\text{-}CH\text{-}CH_3}}{CH}}\text{-}\underset{3}{CH_2}\text{-}\underset{2}{CH_2}\text{-}\underset{1}{COOH}}$$

5-bromo-4-(2-bromo-1-fluoropropyl)-6-fluoroheptanoic acid (PIN)
[not 6-bromo-4-(1-bromo-2-fluoropropyl)-5-fluoroheptanoic acid;
the locant sets are the same in both names, i.e., ‘4,5,6’, but in their order
of appearance in the name the locant set ‘5,4,6’ in the PIN is lower than ‘6,4,5’]

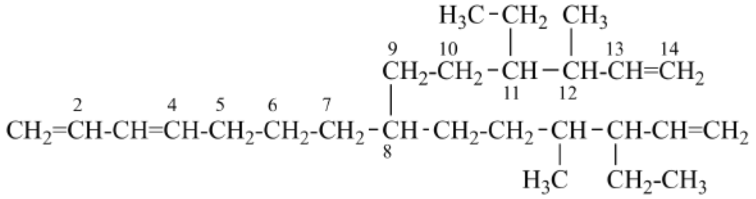
(5)



$$\mathrm{HO{-}\overset{4}{C}H_2{-}\underset{\underset{\displaystyle Br}{|}}{\overset{3}{C}H}{-}\underset{2}{\overset{\overset{\displaystyle \overset{1}{C}OOH}{|}}{C}H}{-}\underset{\underset{\displaystyle OH}{|}}{C}H{-}CH_2{-}Br}$$

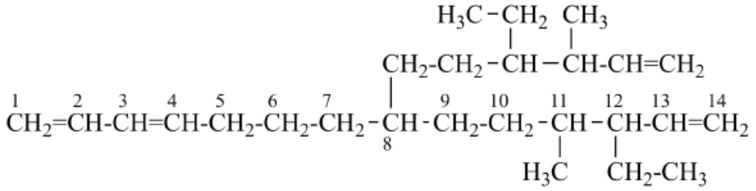
3-bromo-2-(2-bromo-1-hydroxyethyl)-4-hydroxybutanoic acid (PIN)
[not 4-bromo-2-(1-bromo-2-hydroxyethyl)-3-hydroxybutanoic acid;
the locant sets are the same in both names, i.e., ‘2,3,4’, but in their order
of appearance in the name, the locant set ‘3,2,4’ in the PIN is lower than ‘4,2,3’]

(6)



(**I**)

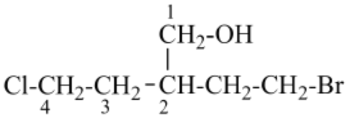
11-ethyl-8-(4-ethyl-3-methylhex-5-en-1-yl)-12-methyltetradeca-1,3,13-triene (PIN) (**I**)



(**II**)

[not 12-ethyl-8-(3-ethyl-4-methylhex-5-en-1-yl)-11-methyltetradeca-1,3,13-triene (**II**)
the locant sets are the same in both names, i.e., ‘8,11,12’, but in their order
of appearance in the name the locant set ‘11,8,12’ in the PIN is lower than ‘12,8,11’]

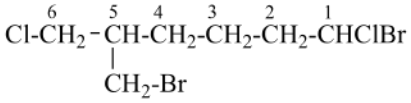
(7)



$$\mathrm{Cl{-}\underset{4}{C}H_2{-}\underset{3}{C}H_2{-}\underset{2}{\overset{\overset{\displaystyle \overset{1}{C}H_2{-}OH}{|}}{C}H}{-}CH_2{-}CH_2{-}Br}$$

2-(2-bromoethyl)-4-chlorobutan-1-ol (PIN)
[not 4-bromo-2-(2-chloroethyl)butan-1-ol
the locant sets are the same in both names, i.e., ‘2,4’ but in the order
of appearance in the name, the locant set ‘2,4’ in the PIN is lower than ‘4,2’]

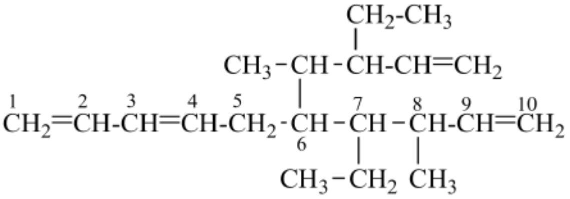
(8)



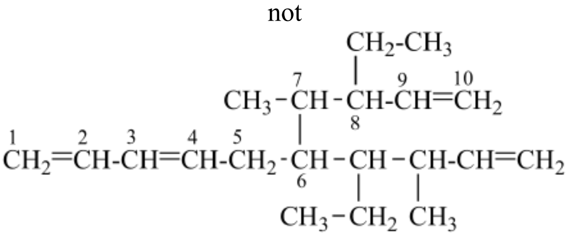
$$\mathrm{Cl{-}\overset{6}{C}H_2{-}\underset{\underset{\displaystyle CH_2{-}Br}{|}}{\overset{5}{C}H}{-}\overset{4}{C}H_2{-}\overset{3}{C}H_2{-}\overset{2}{C}H_2{-}\overset{1}{C}HClBr}$$

1-bromo-5-(bromomethyl)-1,6-dichlorohexane (PIN)
[not 1,6-dibromo-1-chloro-5-(chloromethyl)hexane;
the locant sets are the same in both names, i.e., ‘1,1,5,6’ but in their order
of appearance in the name, the locant set ‘1,5,1,6’ is lower than ‘1,6,1,5’]

(9)

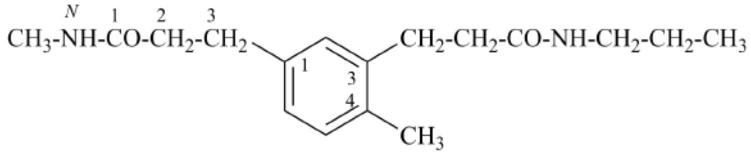


7-ethyl-6-(3-ethylpent-4-en-2-yl)-8-methyldeca-1,3,9-triene (PIN)
not



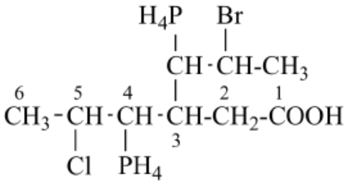
8-ethyl-7-methyl-6-(4-methylhex-5-en-3-yl)deca-1,3,9-triene
[the locant sets are the same in both names, i.e. ‘6,7,8’ but in their order
of appearance in the name, the locant set ‘7,6,8’ is lower than ‘8,7,6’]

(10)



N-methyl-3-{4-methyl-3-[3-oxo-3-(propylamino)propyl]phenyl}propanamide (PIN)
[not 3-{2-methyl-5-[3-(methylamino)-3-oxopropyl]phenyl}-*N*-propylpropanamide;
the locant sets are the same in both names, i.e. '*N*,3' but in their order
of appearance in the name, the locant set '*N*,3' in the PIN is lower than '3,*N*']

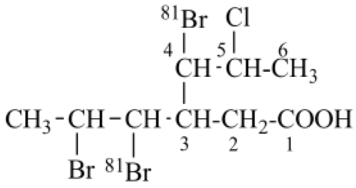
(11)



$$\overset{6}{\mathrm{CH_3}}\text{-}\underset{\mathrm{Cl}}{\overset{5}{\mathrm{CH}}}\text{-}\underset{\mathrm{PH_4}}{\overset{4}{\mathrm{CH}}}\text{-}\underset{3}{\overset{\overset{\mathrm{H_4P}}{\mathrm{CH}}\text{-}\overset{\mathrm{Br}}{\mathrm{CH}}\text{-}\mathrm{CH_3}}{\mathrm{CH}}}\text{-}\overset{2}{\mathrm{CH_2}}\text{-}\overset{1}{\mathrm{COOH}}$$

3-[2-bromo-1-(λ^5-phosphanyl)propyl]-5-chloro-4-(λ^5-phosphanyl)hexanoic acid (PIN)
[not 5-bromo-3-[2-chloro-1-(λ^5-phosphanyl)propyl]-4-(λ^5-phosphanyl)hexanoic acid;
the locant sets are the same in both names, i.e. '3,4,5' but in their order
of appearance in the name, the locant set '3,5,4' in the PIN is lower than '5,3,4']

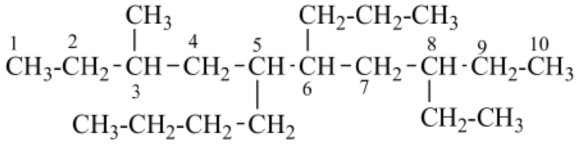
(12)



$$\mathrm{CH_3}\text{-}\underset{\mathrm{Br}}{\mathrm{CH}}\text{-}\underset{\mathrm{^{81}Br}}{\mathrm{CH}}\text{-}\underset{3}{\overset{\overset{4\ \mathrm{^{81}Br}}{\mathrm{CH}}\text{-}\overset{5\ \mathrm{Cl}}{\mathrm{CH}}\text{-}\overset{6}{\mathrm{CH_3}}}{\mathrm{CH}}}\text{-}\underset{2}{\mathrm{CH_2}}\text{-}\underset{1}{\mathrm{COOH}}$$

4-(^{81}Br)bromo-3-[1-(^{81}Br)bromo-2-bromopropyl]-5-chlorohexanoic acid (PIN)
[not 4-(^{81}Br)bromo-5-bromo-3-[1-(^{81}Br)bromo-2-chloropropyl]hexanoic acid;
the locant sets are the same in both names, i.e. '3,4,5' but in their order
of appearance in the name, the locant set '4,3,5' in the PIN is lower than '4,5,3']

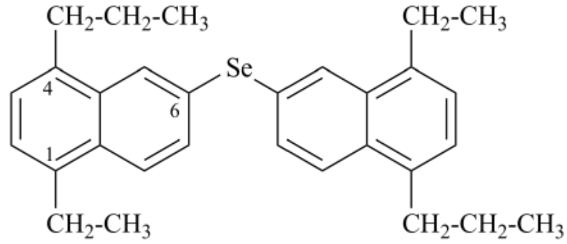
(13)



$$\overset{1}{\mathrm{CH_3}}\text{-}\overset{2}{\mathrm{CH_2}}\text{-}\underset{3}{\overset{\mathrm{CH_3}}{\mathrm{CH}}}\text{-}\overset{4}{\mathrm{CH_2}}\text{-}\underset{\mathrm{CH_3\text{-}CH_2\text{-}CH_2\text{-}CH_2}}{\overset{5}{\mathrm{CH}}}\text{-}\underset{6}{\overset{\mathrm{CH_2\text{-}CH_2\text{-}CH_3}}{\mathrm{CH}}}\text{-}\underset{7}{\mathrm{CH_2}}\text{-}\underset{\mathrm{CH_2\text{-}CH_3}}{\overset{8}{\mathrm{CH}}}\text{-}\overset{9}{\mathrm{CH_2}}\text{-}\overset{10}{\mathrm{CH_3}}$$

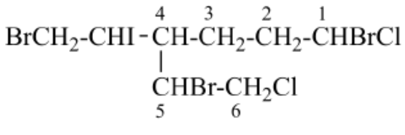
5-butyl-8-ethyl-3-methyl-6-propyldecane (PIN)
[not 6-butyl-3-ethyl-8-methyl-5-propyldecane;
both have the set of locants '3,5,6,8' but
the PIN has them in the order '5,8,3,6' which is lower than '6,3,8,5']

(14)



1-ethyl-6-[(8-ethyl-5-propylnaphthalen-2-yl)selanyl]-4-propylnaphthalene (PIN)
[not 4-ethyl-6-[(5-ethyl-8-propylnaphthalen-2-yl)selanyl]-1-propylnaphthalene:
both have the locant set '1,4,6' but
the PIN set is in the order '1,6,4' which is lower than '4,6,1']

(15)



$$\mathrm{BrCH_2\text{-}CHI}\text{-}\underset{\underset{5\quad\ 6}{\mathrm{CHBr\text{-}CH_2Cl}}}{\overset{4}{\mathrm{CH}}}\text{-}\overset{3}{\mathrm{CH_2}}\text{-}\overset{2}{\mathrm{CH_2}}\text{-}\overset{1}{\mathrm{CHBrCl}}$$

1,5-dibromo-4-(2-bromo-1-iodoethyl)-1,6-dichlorohexane (PIN)
[not 1,6-dibromo-4-(1-bromo-2-chloroethyl)-1-chloro-5-iodohexane;
both have the locant set '1,1,4,5,6' but
the PIN set is in the order '1,5,4,1,6' which is lower than '1,6,4,1,5']

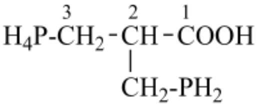
P-45.3 CRITERIA RELATED ONLY TO SUBSTITUENTS WITH NONSTANDARD BONDING NUMBERS, OTHER CRITERIA BEING EQUAL

The following criteria are relative only to substituents with nonstandard bonding numbers applied in turn, until a decision is reached, earlier criteria having been satisfied.

P-45.3.1 the maximum number of substituent group(s) with the higher bonding number cited as prefixes;
P-45.3.2 the lower locant set for substituent group(s) with the higher bonding number cited as prefixes.

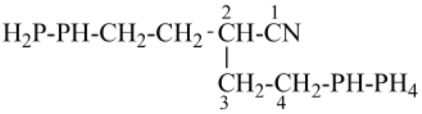
P-45.3.1 The preferred IUPAC name is based on the senior parent structure that has the maximum number of substituent group(s) with the higher bonding number cited as prefixes and directly connected to the parent structure.

Examples:



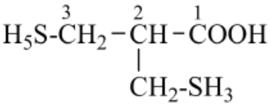
$$H_4P\text{-}\overset{3}{C}H_2\text{-}\overset{2}{C}H(CH_2\text{-}PH_2)\text{-}\overset{1}{C}OOH$$

3-(λ^5-phosphanyl)-2-(phosphanylmethyl)propanoic acid (PIN)
[not 3-phosphanyl-2-(λ^5-phosphanylmethyl)propanoic acid;
the PIN parent structure contains the substituent group having the highest bonding number, 'λ^5' > 'λ^3']



$$H_2P\text{-}PH\text{-}CH_2\text{-}CH_2\text{-}\overset{2}{C}H(\underset{3}{C}H_2\text{-}\underset{4}{C}H_2\text{-}PH\text{-}PH_4)\text{-}\overset{1}{C}N$$

4-(2λ^5-diphosphan-1-yl)-2-(2-diphosphanylethyl)butanenitrile (PIN)
[not 4-diphosphanyl-2-[2-(2λ^5-diphosphan-1-yl)ethyl]butanenitrile;
the PIN parent structure contains the substituent group having the highest bonding number, 'λ^5' > 'λ^3']

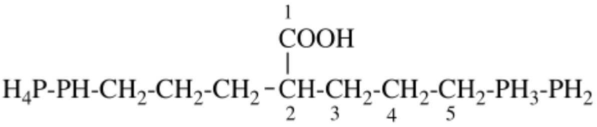


$$H_5S\text{-}\overset{3}{C}H_2\text{-}\overset{2}{C}H(CH_2\text{-}SH_3)\text{-}\overset{1}{C}OOH$$

3-(λ^6-sulfanyl)-2-(λ^4-sulfanylmethyl)propanoic acid (PIN)
[not 3-(λ^4-sulfanyl)-2-(λ^6-sulfanylmethyl)propanoic acid;
the PIN parent structure contains the substituent group having the highest bonding number, 'λ^6' > 'λ^4']

P-45.3.2 The preferred IUPAC name has the lower locant set for substituent group(s) with the higher bonding number(s) cited as prefixes.

Example:



$$H_4P\text{-}PH\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}\underset{2}{C}H(\overset{1}{C}OOH)\text{-}\underset{3}{C}H_2\text{-}\underset{4}{C}H_2\text{-}\underset{5}{C}H_2\text{-}PH_3\text{-}PH_2$$

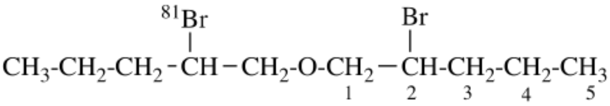
5-(1λ^5-diphosphan-1-yl)-2-[3-(2λ^5-diphosphan-1-yl)propyl]pentanoic acid (PIN)
[not 5-(2λ^5-diphosphan-1-yl)-2-[3-(1λ^5-diphosphan-1-yl)propyl]pentanoic acid]
The locant '1λ^5' for the nonstandard bonding number directly bonded to the parent structure is lower than '2λ^5'.

P-45.4 CRITERIA RELATED ONLY TO ISOTOPIC MODIFICATION OF SUBSTITUENTS

The following criteria are relative only to substituents with isotopic modification applied in turn, until a decision is reached, earlier criteria having been satisfied.

P-45.4.1 The preferred IUPAC name is based on the senior parent structure that has the lowest locant(s) for isotopically modified substituent groups.

Example:



$$CH_3\text{-}CH_2\text{-}CH_2\text{-}CH(^{81}Br)\text{-}CH_2\text{-}O\text{-}\underset{1}{C}H_2\text{-}\underset{2}{C}H(Br)\text{-}\underset{3}{C}H_2\text{-}\underset{4}{C}H_2\text{-}\underset{5}{C}H_3$$

2-bromo-1-{[2-(^{81}Br)bromopentyl]oxy}pentane (PIN)
[not 2-(^{81}Br)bromo-1-[(2-bromopentyl)oxy]pentane]
The isotopically modified substituent for the PIN is attached at '1' which is lower than '2'.

P-45.4.2 The preferred IUPAC name is based on the senior parent structure that has the lowest locant(s) for nuclides of higher atomic number.

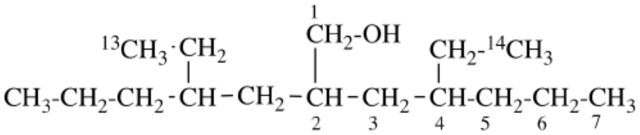
Example:

$$CH_3\text{-}^{18}O\text{-}CH_2\text{-}CH_2\text{-}NH\text{-}\overset{1}{C}H_2\text{-}\overset{2}{C}H_2\text{-}O\text{-}^{13}CH_3$$

2-(^{13}C)methoxy-*N*-[2-[(^{18}O)methoxyethyl]ethan-1-amine (PIN)
[not 2-(^{18}O)methoxy-*N*-[2-(^{13}C)methoxyethyl]ethan-1-amine]
^{18}O > ^{13}C; the ^{18}O isotopically modified substituent for the PIN is attached at '*N*' which is lower than '2'.

P-45.4.3 The preferred IUPAC name is based on the senior parent structure that has the lowest locant(s) for nuclides of higher mass number.

Example:



$$CH_3\text{-}CH_2\text{-}CH_2\text{-}\overset{^{13}CH_3\cdot CH_2}{CH}-CH_2-\underset{2}{\overset{\overset{1}{CH_2\text{-}OH}}{CH}}-\underset{3}{CH_2}-\underset{4}{\overset{CH_2\text{-}^{14}CH_3}{CH}}\text{-}\underset{5}{CH_2}\text{-}\underset{6}{CH_2}\text{-}\underset{7}{CH_3}$$

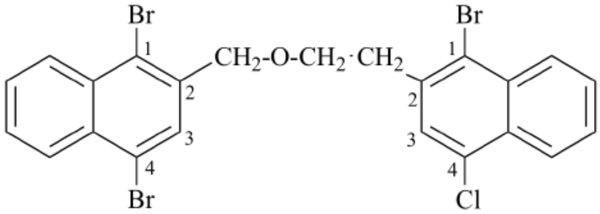
4-[2-^{13}C]ethyl-2-(2-[2-^{14}C]ethylpentyl)heptan-1-ol (PIN)
[not 4-[2-^{14}C]ethyl-2-(2-[2-^{13}C]ethylpentyl)heptan-1-ol
^{14}C > ^{13}C; the ^{14}C isotopically modified substituent for the PIN is attached at ‘2’ which is lower than ‘4’

P-45.5 CRITERIA RELATED TO ALPHANUMERICAL ORDER OF NAMES

The preferred IUPAC name is the name that is earlier in alphanumerical order (see P-14.5). Alphabetic letters are considered first in the order that they appear in the name; all Roman letters are considered before any italic letters, unless the latter are used as locants or are a part of a compound or composite locant, for example, ‘*N*’ and ‘4a’. Then, if still there is a choice, numerical locants are considered in the order of their appearance in the name.

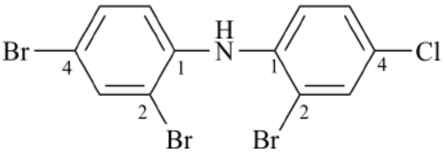
Examples:

(1)



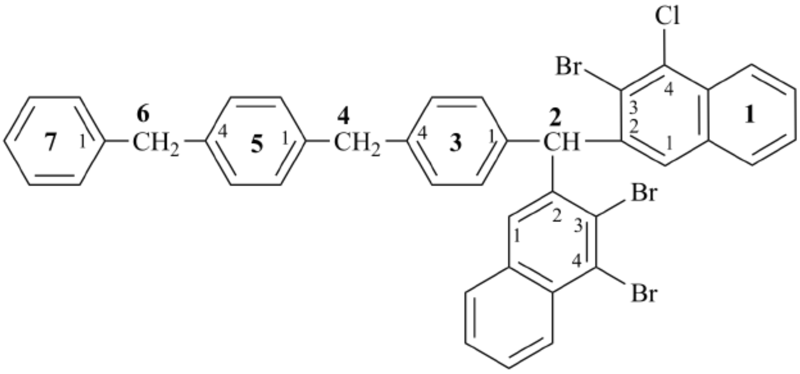
1-bromo-4-chloro-2-{2-[(1,4-dibromonaphthalen-2-yl)methoxy]ethyl}naphthalene (PIN)
[not 1,4-dibromo-2-{[2-(1-bromo-4-chloronaphthalen-2-yl)ethoxy]methyl}naphthalene;
in both names the locant set is ‘1,2,4’, and the locants appear in the name in the same order set ‘1,4,2’ so no decision can be made by P-45.2.2 or P-45.2.3; but ‘bromo’ in the PIN is earlier alphabetically than ‘dibromo’]

(2)



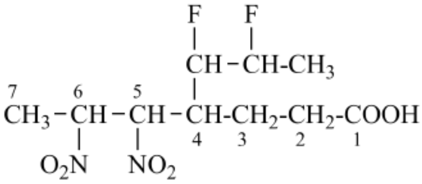
2-bromo-4-chloro-*N*-(2,4-dibromophenyl)aniline (PIN)
[not 2,4-dibromo-*N*-(2-bromo-4-chlorophenyl)aniline;
‘bromo’ in the PIN is earlier alphabetically than ‘dibromo’]

(3)



1^3-bromo-1^4-chloro-2-(3,4-dibromonaphthalen-2-yl)-1(2)-naphthalena-3,5(1,4),7(1)-tribenzenaheptaphane (PIN)
[not 1^3,1^4-dibromo-2-(3-bromo-4-chloronaphthalen-2-yl)-1(2)-naphthalena-3,5(1,4),7(1)-tribenzenaheptaphane;
‘bromo’ in the PIN is earlier alphabetically than ‘dibromo’.]

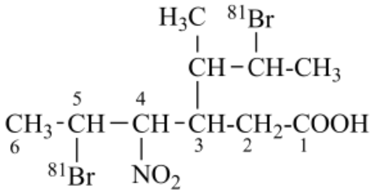
(4)



$$\overset{7}{CH_3}-\underset{O_2N}{\overset{6}{CH}}-\underset{NO_2}{\overset{5}{CH}}-\underset{4}{\overset{\overset{F\quad F}{CH-CH\text{-}CH_3}}{CH}}\text{-}\underset{3}{CH_2}\text{-}\underset{2}{CH_2}\text{-}\underset{1}{COOH}$$

4-(1,2-difluoropropyl)-5,6-dinitroheptanoic acid (PIN)
[not 4-(1,2-dinitropropyl)-5,6-difluoroheptanoic acid;
'difluoro' in the PIN is earlier alphabetically than 'dinitro']

(5)



5-(^{81}Br)bromo-3-[3-(^{81}Br)bromobutan-2-yl]-4-nitrohexanoic acid (PIN)
[not 5-(^{81}Br)bromo-3-[2-(^{81}Br)bromo-1-nitropropyl]-4-methylhexanoic acid;
'bromo-bromo-butanyl' is lower alphanumerically than 'bromo-bromo-nitro']
[**Note:** The 'B' of the element symbol 'Br' is not a factor in the alphabetization]

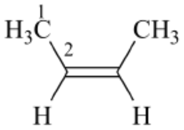
P-45.6 CRITERIA RELATED ONLY TO CONFIGURATION

P-45.6.1 Introduction

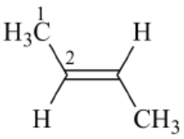
This section is concerned only with the main principles for specification of configuration in names of organic compounds. The spatial structure of an organic compound is systematically indicated by one or more affixes added to a name that does not itself prescribe configuration; such affixes are generally called 'stereodescriptors' and do not change the preferred IUPAC name of a compound established by the principles of nomenclature described in other sections of these recommendations (see P-44 and P-45), under the condition that no choice has yet been encountered during the construction of the preferred IUPAC name. When there is a choice, the preferred IUPAC name must be constructed in conformity with the rules for choosing the principal chain or the senior ring or ring system and also with the priority of the stereodescriptors. Thus, stereoisomers, such as enantiomers and *cis*/*trans* isomers, have names, substitutive or multiplicative, that differ only in the stereodescriptors used. Stereodescriptors describing preferred IUPAC names are all Cahn-Ingold-Prelog CIP descriptors, such as *E*, *Z*, *R*, *S*, *r* and *s* discussed and illustrated in Chapter P-9.

P-45.6.2 General principles. The choice of a parent structure based on the number and location of multiple bonds and double bonds (see P-44.4.1.1, P-44.4.1.2, and P-44.4.1.12) is not configuration dependent. As an example, the configuration of the double bond may be *Z* or *E* in the following alkene that is named according to P-31.1. The names with and without stereodescriptors are the same, i.e. butene. Preferred IUPAC names are generated from the preferred IUPAC name of the alkene when stereodescriptors are correct.

$\underset{1}{\mathrm{C}}\mathrm{H_3}\text{-}\underset{2}{\mathrm{C}}\mathrm{H{=}CH\text{-}CH_3}$
but-2-ene (PIN)



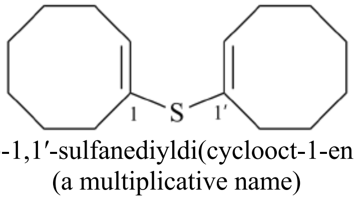
(2*Z*)-but-2-ene (PIN)



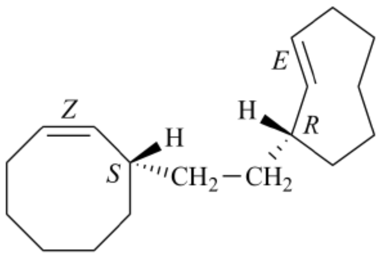
(2*E*)-but-2-ene (PIN)

In contrast, multiplicative names (see P-45.1 and P-15.3) are configuration dependent as shown below. Two different procedures are required: a multiplicative name to describe identical configurations ('*E*' or '*Z*'; or '*R*' or '*S*') in identical units and a substitutive name to describe different configurations ('*E*' and '*Z*' or '*R*' and '*S*') as shown by the first example below.

Example 1:

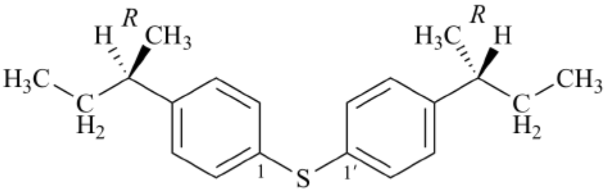


(1*E*,1′*E*)-1,1′-sulfanediyldi(cyclooct-1-ene) (PIN)
(a multiplicative name)

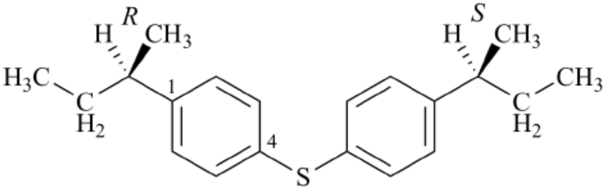

E
Z
H
R
H
S
CH2−CH2

(1*Z*,3*S*)-3-{2-[(1*R*,2*E*)-cyclooct-2-en-1-yl]ethyl}cyclooct-1-ene (PIN)
(1-*cis*,3*S*)-3-{2-[(1*R*,2-*trans*)-cyclooct-2-en-1-yl]ethyl}cyclooct-1-ene
(substitutive names; for the priority of '*Z*' > '*E*' > '*R*' > '*S*', see P-92)

Example 2:

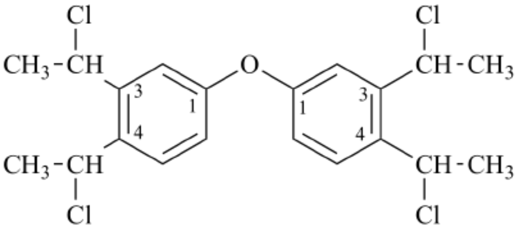

R
H
CH3
H3C
C
H2
1
S
1′
R
H3C
H
CH3
C
H2

1,1′-sulfanediylbis{4-[(2*R*)-butan-2-yl]benzene} (PIN)
(a multiplicative name)

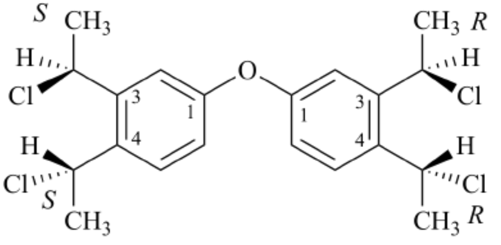

R
H
CH3
H3C
C
H2
1
4
S
S
H
CH3
CH3
C
H2

1-[(2*R*)-butan-2-yl]-4-({4-[(2*S*)-butan-2-yl]phenyl}sulfanyl)benzene (PIN)
(a substitutive name; a multiplicative name is not allowed)
[not 1-[(2*S*)-butan-2-yl]-4-({4-[(2*R*)-butan-2-yl]phenyl}sulfanyl)benzene;
also a substitutive name but since the alphabetic characters and locants
(ignoring the configuration symbols)
are identical the configurational symbols are compared and '*R*' precedes '*S*']

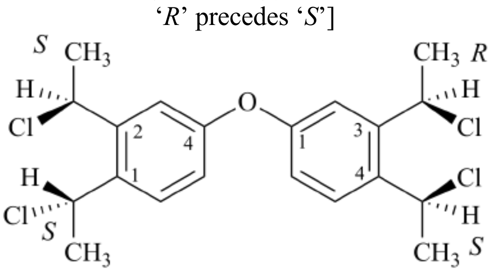
Example 3:


Cl
CH3-CH
3
1
4
CH3-CH
Cl
O
Cl
CH-CH3
1
3
4
CH-CH3
Cl

1,1′-oxybis[3,4-bis(1-chloroethyl)benzene] (PIN)


S
CH3
H
Cl
3
1
4
H
Cl
S
CH3
O
CH3
R
H
Cl
1
3
4
H
Cl
CH3
R

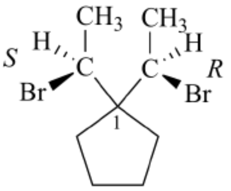
4-{3,4-bis[(1*R*)-1-chloroethyl]phenoxy}-1,2-bis[(1*S*)-1-chloroethyl]benzene (PIN)
[not 4-{3,4-bis[(1*S*)-1-chloroethyl]phenoxy}-1,2-bis[(1*R*)-1-chloroethyl]benzene;
'*R*' precedes '*S*']


S
CH3
H
Cl
2
4
1
H
Cl
S
CH3
O
CH3
R
H
Cl
1
3
4
Cl
H
CH3
S

1,2-bis[(1*S*)-1-chloroethyl]-4-{3-[(1*R*)-1-chloroethyl]-4-[(1*S*)-1-chloroethyl]phenoxy}benzene (PIN)
(a substitutive name; a multiplicative name is not allowed)
[not 4-{3,4-bis[(1*S*)-1-chloroethyl]phenoxy}-2-[(1*R*)-1-chloroethyl]-1-[(1*S*)-1-chloroethyl]benzene;
'1,2,4' is senior to '4,2,1' (see P-45.2.3)]

P-45.6.3 When names based on alphanumerical order and isotopic descriptors are the same, further choice depends on the alphabetic order of the stereochemical descriptors '*R*' and '*S*'.

Example:



1-[(1*R*)-1-bromoethyl]-1-[(1*S*)-1-bromoethyl]cyclopentane (PIN)
[not 1-[(1*S*)-1-bromoethyl]-1-[(1*R*)-1-bromoethyl]cyclopentane;
'*R*' precedes '*S*']

P-46 THE PRINCIPAL CHAIN IN SUBSTITUENT GROUPS

P-46.0 Introduction
P-46.1 The principal substituent chain
P-46.2 Principal substituent chains in isotopically labeled compounds
P-46.3 Principal substituent chains in compounds with stereogenic centers

P-46.0 INTRODUCTION

Compound acyclic substituents, i.e., substituted acyclic substituents, consist of a principal chain and one or more acyclic substituents. If the substituent to the principal chain also has (an) acyclic substituent(s), it itself is a compound substituent; the resulting complete substituent is called a complex acyclic substituent. Complex substituents are named by extending the methods given below for compound substituents.

Compound substituents are named in two ways:

(1) by using alkyl substituents [see P-29.2(1)];

(2) by using alkanyl substituents [see P-29.2(2)].

Alkyl and alkanyl substituent groups have been defined in Section P-29. Simple alkyl substituent groups have their free valence(s) denoted by the suffixes 'yl', 'ylidene' or 'ylidyne' only at position 1. Simple alkanyl substituent groups have their free valence(s) denoted by the suffixes 'yl' or 'ylidene' which may be located at any position of the chain except position 1. Both alkyl and alkanyl substituent groups can form compound substituent groups; for example, CH_3-$C(CH_3)_2$– is 1,1-dimethylethyl, a compound alkyl substituent group, by method (1); and 2-methylpropan-2-yl, a compound alkanyl substituent group, by method (2). In some cases, a compound substituent group resulting from substitution of the principal chain by alkyl or alkanyl substituent groups results in the same structure that corresponds to a simple alkanyl substituent group; for example, CH_3-CH_2-CH_2-CH_2-$CH(CH_3)$– is 1-methylpentyl by method (1), but hexan-2- yl by method (2).

P-46.1 THE PRINCIPAL SUBSTITUENT CHAIN

Selection of the principal chain of a compound substituent is accomplished in accordance with the following criteria, applied successively in the order given until a decision is reached. They are listed here and illustrated in P-46.1.1 through P-46.1.13. The principal substituent chain has:

(a) the greater number of heteroatoms; this criterion is used only in method (2) in P-46.0;

(b) the greater number of skeletal atoms, i.e., the longest chain;

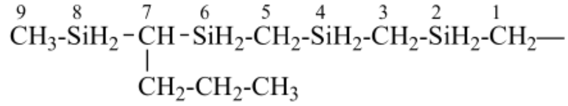
In acyclic substituents the order of seniority between unsaturation and length of chain given in earlier recommendations is reversed. Thus, the first criterion to be considered in choosing a preferred acyclic substituent is the length of the chain; unsaturation is now a lower criterion [see (d)].

(c) the greater number of heteroatoms in the order: O > S > Se > Te > N > P > As > Sb > Bi > Si > Ge > Sn > Pb > B > Al > Ga > In > Tl;
(d) the greater number of multiple bonds regardless of type, then the greater number of double bonds;
(e) one or more atoms with nonstandard bonding numbers;
(f) the lowest locants for heteroatoms; this criterion is used only in method (2) in P-46.0;
(g) the lowest locants for heteroatoms appearing first in the order: O > S > Se > Te > N > P > As > Sb > Bi > Si > Ge > Sn > Pb > B > Al > Ga > In > Tl;
(h) the lowest locants for free valences of any kind ('yl', 'ylidene', 'ylidyne');
(i) the lowest locant(s) for multiple bonds, regardless of type, then the lower locant(s) for double bonds;
(j) the lowest locant(s) for (an) atom(s) with nonstandard bonding number(s);
(k) the greatest number of substituents of any kind; this criterion is applicable to both methods (1) and (2) in P-46.0;

(l) the lowest locants for substituents; this criterion is applicable to both methods (1) and (2) in P-46.0;
(m) the lowest locants for the substituent(s) cited earlier in alphanumerical order; this criterion is applicable to both methods (1) and (2) in P-46.0.

P-46.1.1 The principal substituent chain has the greater number of heteroatoms [criterion (a) in P-46.1]; this criterion is used only in method (2) of P-46.0.

Example:

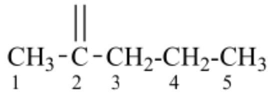


$\mathrm{\overset{9}{C}H_3\text{-}\overset{8}{Si}H_2\text{-}\overset{7}{C}H(CH_2\text{-}CH_2\text{-}CH_3)\text{-}\overset{6}{Si}H_2\text{-}\overset{5}{C}H_2\text{-}\overset{4}{Si}H_2\text{-}\overset{3}{C}H_2\text{-}\overset{2}{Si}H_2\text{-}\overset{1}{C}H_2\text{—}}$

7-propyl-2,4,6,8-tetrasilanonan-1-yl (preferred prefix)
[not 7-(methylsilyl)-2,4,6-trisiladecan-1-yl]

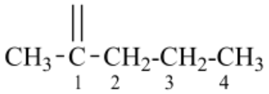
P-46.1.2 The principal substituent chain has the greater number of skeletal atoms, i.e., the longest chain [criterion (b) in P-46.1]. This criterion is applicable to both methods (1) and (2) of P-46.0; both methods generate simple and compound substituent groups.

Examples:



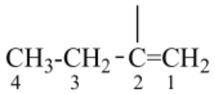
$\mathrm{\underset{1}{C}H_3\text{-}\underset{2}{\overset{\|}{C}}\text{-}\underset{3}{C}H_2\text{-}\underset{4}{C}H_2\text{-}\underset{5}{C}H_3}$

(2) pentan-2-ylidene (preferred prefix)
(a simple substituent group)



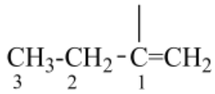
$\mathrm{CH_3\text{-}\underset{1}{\overset{\|}{C}}\text{-}\underset{2}{C}H_2\text{-}\underset{3}{C}H_2\text{-}\underset{4}{C}H_3}$

(1) 1-methylbutylidene
(a compound substituent group)



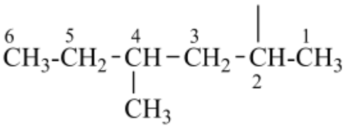
$\mathrm{\underset{4}{C}H_3\text{-}\underset{3}{C}H_2\text{-}\underset{2}{\overset{|}{C}}\text{=}\underset{1}{C}H_2}$

(2) but-1-en-2-yl (preferred prefix)
(a simple substituent group)



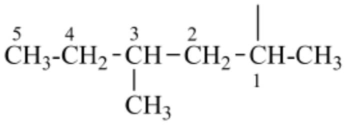
$\mathrm{\underset{3}{C}H_3\text{-}\underset{2}{C}H_2\text{-}\underset{1}{\overset{|}{C}}\text{=}CH_2}$

(1) 1-methylidenepropyl
(a compound substituent group)



$\mathrm{\overset{6}{C}H_3\text{-}\overset{5}{C}H_2\text{-}\overset{4}{C}H(CH_3)\text{-}\overset{3}{C}H_2\text{-}\underset{2}{\overset{|}{C}}H\text{-}\overset{1}{C}H_3}$

(2) 4-methylhexan-2-yl (preferred prefix)
(a compound substituent group)

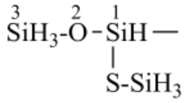


$\mathrm{\overset{5}{C}H_3\text{-}\overset{4}{C}H_2\text{-}\overset{3}{C}H(CH_3)\text{-}\overset{2}{C}H_2\text{-}\underset{1}{\overset{|}{C}}H\text{-}CH_3}$

(1) 1,3-dimethylpentyl
(a compound substituent group)

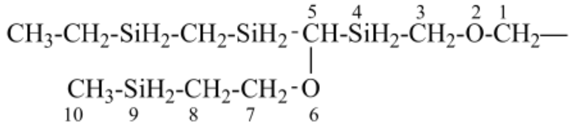
P-46.1.3 The principal substituent chain has the greater number of heteroatoms in the order: O > S > Se > Te > N > P > As > Sb > Bi > Si > Ge > Sn > Pb > B > Al > Ga > In > Tl [criterion (c) in P-46.1].

Examples:



$\mathrm{\overset{3}{Si}H_3\text{-}\overset{2}{O}\text{-}\overset{1}{Si}H(S\text{-}SiH_3)\text{—}}$

1-(silylsulfanyl)disiloxanyl (preselected prefix)
[not 1-(silyloxy)disilathianyl; ‘O’ > ‘S’]

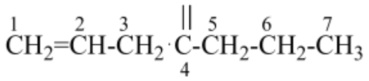


$\mathrm{CH_3\text{-}CH_2\text{-}SiH_2\text{-}CH_2\text{-}SiH_2\text{-}\overset{5}{C}H(\overset{6}{O}\text{-}\overset{7}{C}H_2\text{-}\overset{8}{C}H_2\text{-}\overset{9}{Si}H_2\text{-}\overset{10}{C}H_3)\text{-}\overset{4}{Si}H_2\text{-}\overset{3}{C}H_2\text{-}\overset{2}{O}\text{-}\overset{1}{C}H_2\text{—}}$

5-{[(ethylsilyl)methyl]silyl}-2,6-dioxa-4,9-disiladecan-1-yl (preferred prefix)
[not 5-[2-(methylsilyl)ethoxy]-2-oxa-4,6,8-trisiladecan-1-yl;
two oxygens are senior to one oxygen]

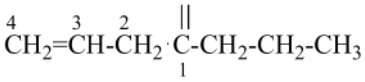
P-46.1.4 The principal chain has the greater number of multiple bonds regardless of type, then the greater number of double bonds [criterion (d) in P-46.1]; this criterion is applicable to methods (1) and (2) in P-46.0; both generate simple and compound substituent groups.

Examples:



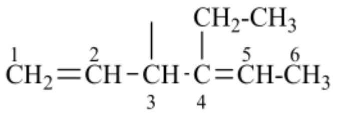
$\mathrm{\overset{1}{C}H_2\text{=}\overset{2}{C}H\text{-}\overset{3}{C}H_2\text{-}\underset{4}{\overset{\|}{C}}\text{-}\overset{5}{C}H_2\text{-}\overset{6}{C}H_2\text{-}\overset{7}{C}H_3}$

(2) hept-1-en-4-ylidene (preferred prefix)
(a simple substituent group)



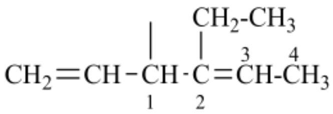
$\mathrm{\overset{4}{C}H_2\text{=}\overset{3}{C}H\text{-}\overset{2}{C}H_2\text{-}\underset{1}{\overset{\|}{C}}\text{-}CH_2\text{-}CH_2\text{-}CH_3}$

(1) 1-propylbut-3-en-1-ylidene
(a compound substituent group)



$\overset{1}{C}H_2{=}\overset{2}{C}H\text{-}\underset{3}{\overset{|}{C}H}\text{-}\underset{4}{\overset{CH_2\text{-}CH_3}{\overset{|}{C}}}{=}\overset{5}{C}H\text{-}\overset{6}{C}H_3$

(2) 4-ethylhexa-1,4-dien-3-yl
(preferred prefix; a compound substituent group)

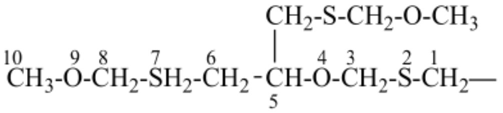


$CH_2{=}CH\text{-}\underset{1}{\overset{|}{C}H}\text{-}\underset{2}{\overset{CH_2\text{-}CH_3}{\overset{|}{C}}}{=}\overset{3}{C}H\text{-}\overset{4}{C}H_3$

(1) 1-ethenyl-2-ethylbut-2-en-1-yl
(a compound substituent group)

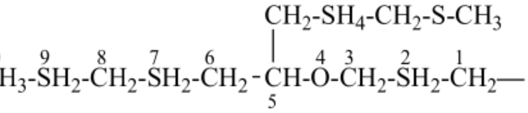
P-46.1.5 The principal substituent chain has one or more atoms with nonstandard bonding numbers [criterion (e) in P-46.1]. When a choice is needed between two substituent chains having skeletal atoms with nonstandard bonding numbers, the one having the maximum number of atoms with nonstandard bonding numbers is chosen as principal substituent chain. If a further choice is needed between the same skeletal atom with different nonstandard bonding numbers, preference for the principal substituent chain is given in order of the decreasing numerical value of the bonding number, i.e., λ^6 is senior to λ^4.

Examples:



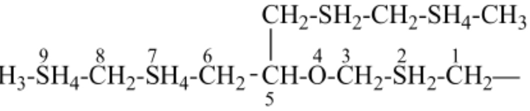
$\overset{10}{C}H_3\text{-}\overset{9}{O}\text{-}\overset{8}{C}H_2\text{-}\overset{7}{S}H_2\text{-}\overset{6}{C}H_2\text{-}\underset{5}{\overset{CH_2\text{-}S\text{-}CH_2\text{-}O\text{-}CH_3}{\overset{|}{C}H}}\text{-}\overset{4}{O}\text{-}\overset{3}{C}H_2\text{-}\overset{2}{S}\text{-}\overset{1}{C}H_2\text{—}$

5-{[(methoxymethyl)sulfanyl]methyl}-4,9-dioxa-2,7λ^4-dithiadecan-1-yl (preferred prefix)
[not 5-{[(methoxymethyl)-λ^4-sulfanyl]methyl}-4,9-dioxa-2,7-dithiadecan-1-yl;
one nonstandard bonding atom *vs.* zero]



$\overset{10}{C}H_3\text{-}\overset{9}{S}H_2\text{-}\overset{8}{C}H_2\text{-}\overset{7}{S}H_2\text{-}\overset{6}{C}H_2\text{-}\underset{5}{\overset{CH_2\text{-}SH_4\text{-}CH_2\text{-}S\text{-}CH_3}{\overset{|}{C}H}}\text{-}\overset{4}{O}\text{-}\overset{3}{C}H_2\text{-}\overset{2}{S}H_2\text{-}\overset{1}{C}H_2\text{—}$

5-({[(methylsulfanyl)methyl]-λ^6-sulfanyl}methyl)-4-oxa-2λ^4,7λ^4,9λ^4-trithiadecan-1-yl (preferred prefix)
[not 5-({[(methyl-λ^4-sulfanyl)methyl]-λ^4-sulfanyl}methyl)-4-oxa-2λ^4,7λ^6,9-trithiadecan-1-yl;
three nonstandard bonding atoms *vs.* two]



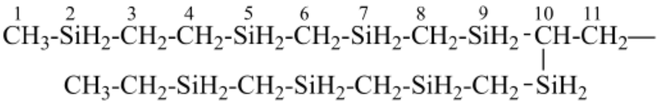
$\overset{10}{C}H_3\text{-}\overset{9}{S}H_4\text{-}\overset{8}{C}H_2\text{-}\overset{7}{S}H_4\text{-}\overset{6}{C}H_2\text{-}\underset{5}{\overset{CH_2\text{-}SH_2\text{-}CH_2\text{-}SH_4\text{-}CH_3}{\overset{|}{C}H}}\text{-}\overset{4}{O}\text{-}\overset{3}{C}H_2\text{-}\overset{2}{S}H_2\text{-}\overset{1}{C}H_2\text{—}$

5-({[(methyl-λ^6-sulfanyl)methyl]-λ^4-sulfanyl}methyl)-4-oxa-2λ^4,7λ^6,9λ^6-trithiadecan-1-yl (preferred prefix)
[not 5-({[(methyl-λ^6-sulfanyl)methyl]-λ^6-sulfanyl }methyl)-4-oxa-2λ^4,7λ^4,9λ^6-trithiadecan-1-yl;
two λ^6 nonstandard bonding atoms and one λ^4 nonstandard bonding atoms *vs.*
two λ^4 and one λ^6 nonstandard bonding atoms]

P-46.1.6 The principal substituent chain has the lowest locants for heteroatoms [criterion (f) in P-46.1]; this criterion is used only in method (2) of P-46.0.

This is a change. Heteroatoms in chains are now considered as part of the parent hydride; as such they have seniority over suffixes for numbering (see P-14.4; see also P-15.4.3); this change makes ‘a’ terms nondetachable in skeletal replacement in chains, rings, and ring systems.

Example:

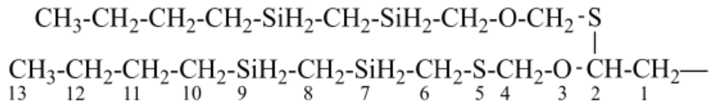


$\overset{1}{C}H_3\text{-}\overset{2}{Si}H_2\text{-}\overset{3}{C}H_2\text{-}\overset{4}{C}H_2\text{-}\overset{5}{Si}H_2\text{-}\overset{6}{C}H_2\text{-}\overset{7}{Si}H_2\text{-}\overset{8}{C}H_2\text{-}\overset{9}{Si}H_2\text{-}\underset{CH_3\text{-}CH_2\text{-}SiH_2\text{-}CH_2\text{-}SiH_2\text{-}CH_2\text{-}SiH_2\text{-}CH_2\text{-}SiH_2}{\underset{|}{\overset{10}{C}H}}\text{-}\overset{11}{C}H_2\text{—}$

10-(1,3,5,7-tetrasilanonan-1-yl)-2,5,7,9-tetrasilaundecan-11-yl (preferred prefix)
[not 10-(1,3,5,8-tetrasilanonan-1-yl)-3,5,7,9-tetrasilaundecan-11-yl;
the locant set in the principal substituent chain ‘2,5,7,9’ is lower than the set ‘3,5,7,9’]

P-46.1.7 The principal substituent chain has the lowest locants for heteroatoms appearing first in the order: O > S > Se > Te > N > P > As > Sb > Bi > Si > Ge > Sn > Pb > B > Al > Ga > In > Tl [criterion(g) in P-46.1]; this criterion is used only in method (2) of P-46.0.

Example:

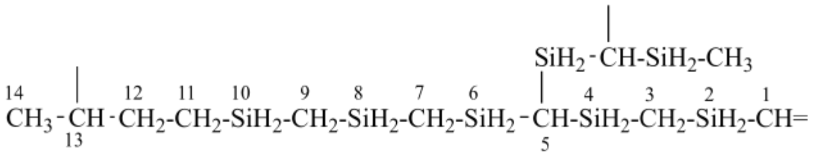


$\underset{13}{C}H_3\text{-}\underset{12}{C}H_2\text{-}\underset{11}{C}H_2\text{-}\underset{10}{C}H_2\text{-}\underset{9}{Si}H_2\text{-}\underset{8}{C}H_2\text{-}\underset{7}{Si}H_2\text{-}\underset{6}{C}H_2\text{-}\underset{5}{S}\text{-}\underset{4}{C}H_2\text{-}\underset{3}{O}\text{-}\underset{2}{\overset{CH_3\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}SiH_2\text{-}CH_2\text{-}SiH_2\text{-}CH_2\text{-}O\text{-}CH_2\text{-}S}{\overset{|}{C}H}}\text{-}\underset{1}{C}H_2\text{—}$

2-{[({[(butylsilyl)methyl]silyl}methoxy)methyl]sulfanyl}-3-oxa-5-thia-7,9-disilatridecan-1-yl (preferred prefix)
[not 2-{[({[(butylsilyl)methyl]silyl}methyl)sulfanyl]methoxy}-5-oxa-3-thia-7,9-disilatridecan-1-yl;
‘3-oxa’ is senior to ‘5-oxa’]

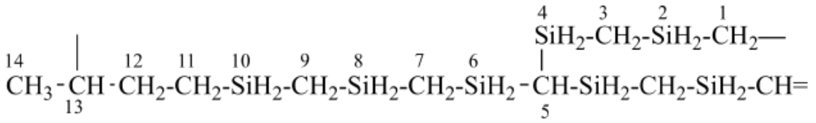
P-46.1.8 The principal substituent chain has the lowest locants for free valences of any kind in the order ‘yl’ > ‘ylidene’ > ‘ylidyne’ [criterion (h) in P-46.1].

Examples:



$$\begin{array}{l}\mathrm{SiH_2\text{-}CH\text{-}SiH_2\text{-}CH_3}\\ \mathrm{CH_3\text{-}CH\text{-}CH_2\text{-}CH_2\text{-}SiH_2\text{-}CH_2\text{-}SiH_2\text{-}CH_2\text{-}SiH_2\text{-}CH\text{-}SiH_2\text{-}CH_2\text{-}SiH_2\text{-}CH{=}}\end{array}$$

5-{[(methylsilyl)ylomethyl]silyl}-2,4,6,8,10-pentasilatetradecan-13-yl-1-ylidene (preferred prefix)

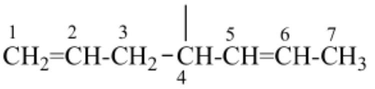


$$\begin{array}{l}\mathrm{SiH_2\text{-}CH_2\text{-}SiH_2\text{-}CH_2\text{—}}\\ \mathrm{CH_3\text{-}CH\text{-}CH_2\text{-}CH_2\text{-}SiH_2\text{-}CH_2\text{-}SiH_2\text{-}CH_2\text{-}SiH_2\text{-}CH\text{-}SiH_2\text{-}CH_2\text{-}SiH_2\text{-}CH{=}}\end{array}$$

5-{[(diylomethylsilyl)methyl]silyl}-2,4,6,8,10-pentasilatetradecane-1,13-diyl (preferred prefix)
(for 'ylo' as a prefix, see P-70.3.1, P-71.5)

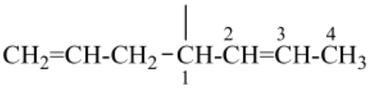
P-46.1.9 The principal substituent chain has the lowest locant(s) for multiple bonds, regardless of type, then the lowest locant(s) for double bonds [criterion (i) in P-46.1]. This criterion is applicable to both methods (1) and (2) in P-46.0; both methods generate simple and compound substituent groups.

Examples:



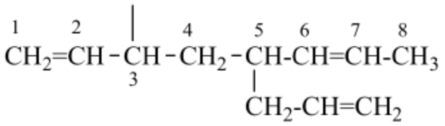
$$\mathrm{CH_2{=}CH\text{-}CH_2\text{-}CH\text{-}CH{=}CH\text{-}CH_3}$$

(2) hepta-1,5-dien-4-yl (preferred prefix)
(a simple substituent group)



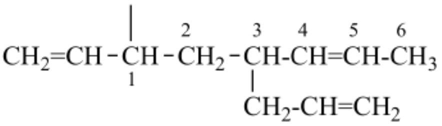
$$\mathrm{CH_2{=}CH\text{-}CH_2\text{-}CH\text{-}CH{=}CH\text{-}CH_3}$$

(1) 1-(prop-2-en-1-yl)but-2-en-1-yl
(a compound substituent group)



$$\begin{array}{l}\mathrm{CH_2{=}CH\text{-}CH\text{-}CH_2\text{-}CH\text{-}CH{=}CH\text{-}CH_3}\\ \mathrm{CH_2\text{-}CH{=}CH_2}\end{array}$$

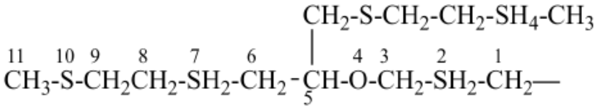
(2) 5-(prop-2-en-1-yl)octa-1,6-dien-3-yl (preferred prefix)
(a compound substituent group)



$$\begin{array}{l}\mathrm{CH_2{=}CH\text{-}CH\text{-}CH_2\text{-}CH\text{-}CH{=}CH\text{-}CH_3}\\ \mathrm{CH_2\text{-}CH{=}CH_2}\end{array}$$

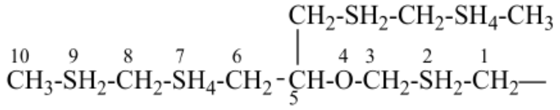
(1) 1-ethenyl-3-(prop-2-en-1-yl)hex-4-en-1-yl
(a compound substituent group)

P-46.1.10 The principal substituent chain has the lowest locant(s) for (an) atom(s) with nonstandard bonding number(s) [criterion (j) in P-46.1]. If a further choice is needed, the principal substituent chain has (an) atom(s) of the higher bonding number with the lowest locant.
Examples:



$$\begin{array}{l}\mathrm{CH_2\text{-}S\text{-}CH_2\text{-}CH_2\text{-}SH_4\text{-}CH_3}\\ \mathrm{CH_3\text{-}S\text{-}CH_2CH_2\text{-}SH_2\text{-}CH_2\text{-}CH\text{-}O\text{-}CH_2\text{-}SH_2\text{-}CH_2\text{—}}\end{array}$$

5-({[2-(methyl-λ^6-sulfanyl)ethyl]sulfanyl}methyl)-4-oxa-2λ^4,7λ^4,10-trithiaundecan-1-yl (preferred prefix)
[not 5-({[(methylsulfanyl)ethyl]-λ^4-sulfanyl}methyl)-4-oxa-2λ^4,7,10λ^6-trithiaundecan-1-yl;
the locant set for the nonstandard bonding atoms '2,7' is lower than '2,10']

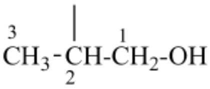


$$\begin{array}{l}\mathrm{CH_2\text{-}SH_2\text{-}CH_2\text{-}SH_4\text{-}CH_3}\\ \mathrm{CH_3\text{-}SH_2\text{-}CH_2\text{-}SH_4\text{-}CH_2\text{-}CH\text{-}O\text{-}CH_2\text{-}SH_2\text{-}CH_2\text{—}}\end{array}$$

5-({[(methyl-λ^6-sulfanyl)methyl]-λ^4-sulfanyl}methyl)-4-oxa-2λ^4,7λ^6,9λ^4-trithiadecan-1-yl (preferred prefix)
[not 5-({[(methyl-λ^4-sulfanyl)methyl]-λ^6-sulfanyl}methyl)-4-oxa-2λ^4,7λ^4,9λ^6-trithiadecan-1-yl;
the λ^6 nonstandard bonding atom in the PIN name is at position '7' which is lower than '9']

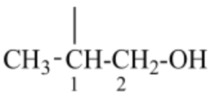
P-46.1.11 The principal substituent chain has the greatest number of substituents of any kind [criterion (k) in P-46.1]. This criterion is applicable to both methods (1) and (2) in P-46.0; both methods generate compound and complex substituent groups, respectively.

When applicable, the principal substituent chain has the greatest number of substituent groups with the highest bonding number. When method (2) is applied, numbering is based on low locants for substituents with atoms with the highest bonding number [P-14.4 (h)].
Examples:



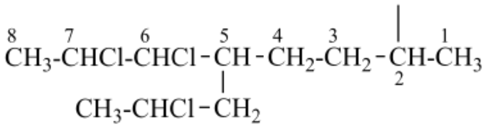
$$\mathrm{CH_3\text{-}CH\text{-}CH_2\text{-}OH}$$

(2) 1-hydroxypropan-2-yl (preferred prefix)
(a compound substituent group)



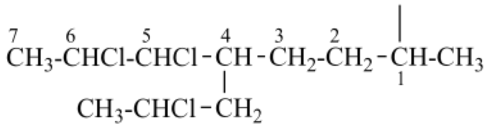
$$\mathrm{CH_3\text{-}CH\text{-}CH_2\text{-}OH}$$

(1) 2-hydroxy-1-methylethyl
(a compound substituent group)
[not 1-(hydroxymethyl)ethyl]



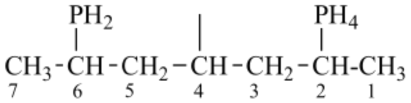
$$\mathrm{\overset{8}{CH_3}-\overset{7}{CHCl}-\overset{6}{CHCl}-\overset{5}{\underset{CH_3-CHCl-CH_2}{CH}}-\overset{4}{CH_2}-\overset{3}{CH_2}-\underset{2}{\overset{|}{CH}}-\overset{1}{CH_3}}$$

(2) 6,7-dichloro-5-(2-chloropropyl)octan-2-yl
(preferred prefix)
[not 7-chloro-5-(1,2-dichloropropyl)octan-2-yl;
a complex substituent group]



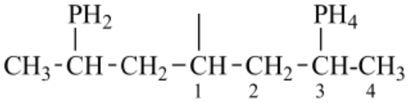
$$\mathrm{\overset{7}{CH_3}-\overset{6}{CHCl}-\overset{5}{CHCl}-\overset{4}{\underset{CH_3-CHCl-CH_2}{CH}}-\overset{3}{CH_2}-\overset{2}{CH_2}-\underset{1}{\overset{|}{CH}}-CH_3}$$

(1) 5,6-dichloro-4-(2-chloropropyl)-1-methylheptyl
(a complex substituent group)



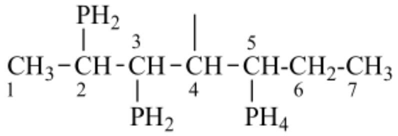
$$\mathrm{\underset{7}{CH_3}-\underset{6}{\overset{PH_2}{CH}}-\underset{5}{CH_2}-\underset{4}{\overset{|}{CH}}-\underset{3}{CH_2}-\underset{2}{\overset{PH_4}{CH}}-\underset{1}{CH_3}}$$

(2) 2-(λ^5-phosphanyl)-6-phosphanylheptan-4-yl
(preferred prefix)
(a compound substituent group)



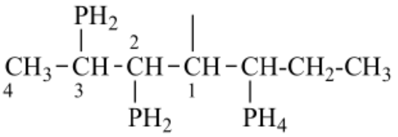
$$\mathrm{CH_3-\overset{PH_2}{CH}-CH_2-\underset{1}{\overset{|}{CH}}-\underset{2}{CH_2}-\underset{3}{\overset{PH_4}{CH}}-\underset{4}{CH_3}}$$

(1) 3-(λ^5-phosphanyl)-1-(2-phosphanylpropyl)butyl
(a complex substituent group)



$$\mathrm{\underset{1}{CH_3}-\underset{2}{\overset{PH_2}{CH}}-\overset{3}{\underset{PH_2}{CH}}-\underset{4}{\overset{|}{CH}}-\overset{5}{\underset{PH_4}{CH}}-\underset{6}{CH_2}-\underset{7}{CH_3}}$$

(2) 5-(λ^5-phosphanyl)-2,3-bis(phosphanyl)heptan-4-yl
(preferred prefix)
(a compound substituent group)



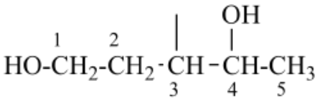
$$\mathrm{\underset{4}{CH_3}-\underset{3}{\overset{PH_2}{CH}}-\overset{2}{\underset{PH_2}{CH}}-\underset{1}{\overset{|}{CH}}-\underset{PH_4}{CH}-CH_2-CH_3}$$

(1) 2,3-bis(phosphanyl)-1-[1-(λ^5-phosphanyl)propyl]butyl
(a complex substituent group)

P-46.1.12 The principal chain has the lowest locants for substituents [criterion (l) in P-46.1]. This criterion is applicable to both methods (1) and (2) of P-46.0; both methods generate compound and complex substituent groups.

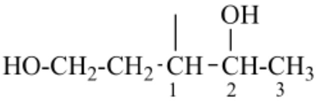
When applicable, the principal substituent chain has the greatest number of substituent groups with (an) atom(s) of the highest bonding number. When method (2) is applied, numbering is based on low locants for substituents with atoms with the highest bonding number [P-14.4 (h)].

Examples:



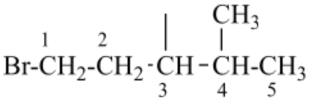
$$\mathrm{HO-\overset{1}{CH_2}-\overset{2}{CH_2}-\underset{3}{\overset{|}{CH}}-\underset{4}{\overset{OH}{CH}}-\underset{5}{CH_3}}$$

(2) 1,4-dihydroxypentan-3-yl (preferred prefix)
(a compound substituent group)



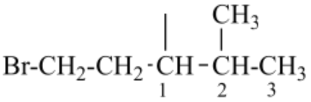
$$\mathrm{HO-CH_2-CH_2-\underset{1}{\overset{|}{CH}}-\underset{2}{\overset{OH}{CH}}-\underset{3}{CH_3}}$$

(1) 2-hydroxy-1-(2-hydroxyethyl)propyl
(a complex substituent group)
[not 3-hydroxy-1-(1-hydroxyethyl)propyl;
the locant set ‘1,2’ is lower than ‘1,3‘]



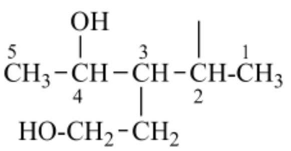
$$\mathrm{Br-\overset{1}{CH_2}-\overset{2}{CH_2}-\underset{3}{\overset{|}{CH}}-\underset{4}{\overset{CH_3}{CH}}-\underset{5}{CH_3}}$$

(2) 1-bromo-4-methylpentan-3-yl (preferred prefix)
(a compound substituent group)



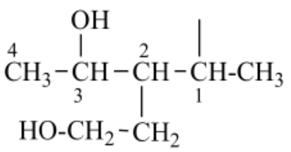
$$\mathrm{Br-CH_2-CH_2-\underset{1}{\overset{|}{CH}}-\underset{2}{\overset{CH_3}{CH}}-\underset{3}{CH_3}}$$

(1) 1-(2-bromoethyl)-2-methylpropyl
(a complex substituent group)



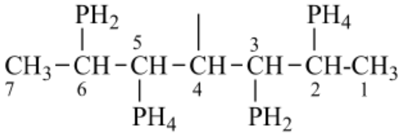
$$\mathrm{\overset{5}{CH_3}-\underset{4}{\overset{OH}{CH}}-\overset{3}{\underset{HO-CH_2-CH_2}{CH}}-\underset{2}{\overset{|}{CH}}-\overset{1}{CH_3}}$$

(2) 4-hydroxy-3-(2-hydroxyethyl)pentan-2-yl (preferred prefix)
(a complex substituent group)



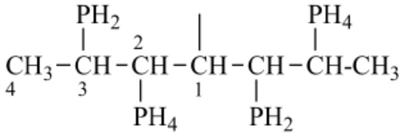
$$\mathrm{\overset{4}{CH_3}-\underset{3}{\overset{OH}{CH}}-\overset{2}{\underset{HO-CH_2-CH_2}{CH}}-\underset{1}{\overset{|}{CH}}-CH_3}$$

(1) 3-hydroxy-2-(2-hydroxyethyl)-1-methylbutyl
(a complex substituent group)



$$\mathrm{\underset{7}{CH_3}-\underset{6}{\overset{PH_2}{CH}}-\overset{5}{\underset{PH_4}{CH}}-\underset{4}{\overset{|}{CH}}-\overset{3}{\underset{PH_2}{CH}}-\underset{2}{\overset{PH_4}{CH}}-\underset{1}{CH_3}}$$

(2) 2,5-bis(λ^5-phosphanyl)-3,6-bis(phosphanyl)heptan-4-yl
(preferred prefix)
[not 3,6-bis(λ^5-phosphanyl)-2,5-bis(phospanyl)heptan-4-yl;
the locant set ‘2,5’ is lower than ‘3,6’]

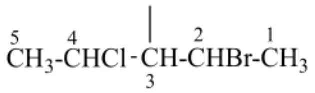


$$\mathrm{\underset{4}{CH_3}-\underset{3}{\overset{PH_2}{CH}}-\overset{2}{\underset{PH_4}{CH}}-\underset{1}{\overset{|}{CH}}-\underset{PH_2}{CH}-\overset{PH_4}{CH}-CH_3}$$

(1) 2-(λ^{5}phosphanyl)-3-phosphanyl-1-[2-(λ^{5}phosphanyl)-1-phosphanylpropyl]butyl
(a complex substituent group)

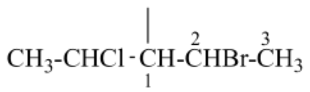
P-46.1.13 The principal substituent chain has the lowest locants for the substituent(s) cited earlier in alphanumerical order [criterion (m) in P-46.1]; this criterion is applicable to both methods (1) and (2) in P-46.0; both methods generate compound and complex substituent groups.

Examples:



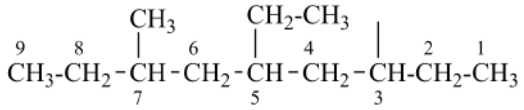
$$\overset{5}{C}H_3\text{-}\overset{4}{C}HCl\text{-}\underset{3}{\overset{|}{C}}H\text{-}\overset{2}{C}HBr\text{-}\overset{1}{C}H_3$$

(2) 2-bromo-4-chloropentan-3-yl (preferred prefix)
(a compound substituent group)
(not 4-bromo-2-chloropentan-3-yl;
‘2-bromo’ is senior to ‘4-bromo’)



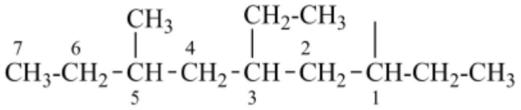
$$CH_3\text{-}CHCl\text{-}\underset{1}{\overset{|}{C}}H\text{-}\overset{2}{C}HBr\text{-}\overset{3}{C}H_3$$

(1) 2-bromo-1-(1-chloroethyl)propyl
(a complex substituent group)
[not 1-(1-bromoethyl)-2-chloropropyl;
‘bromo...chloro’ is senior to ‘bromoethyl’]



$$\overset{9}{C}H_3\text{-}\overset{8}{C}H_2\text{-}\underset{7}{\overset{CH_3}{C}}H\text{-}\overset{6}{C}H_2\text{-}\underset{5}{\overset{CH_2\text{-}CH_3}{C}}H\text{-}\overset{4}{C}H_2\text{-}\underset{3}{\overset{|}{C}}H\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}H_3$$

(2) 5-ethyl-7-methylnonan-3-yl (preferred prefix)
(a compound substituent group)



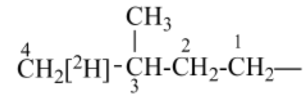
$$\overset{7}{C}H_3\text{-}\overset{6}{C}H_2\text{-}\underset{5}{\overset{CH_3}{C}}H\text{-}\overset{4}{C}H_2\text{-}\underset{3}{\overset{CH_2\text{-}CH_3}{C}}H\text{-}\overset{2}{C}H_2\text{-}\underset{1}{\overset{|}{C}}H\text{-}CH_2\text{-}CH_3$$

(1) 1,3-diethyl-5-methylheptyl
(a compound substituent group)

P-46.2 PRINCIPAL SUBSTITUENT CHAINS IN ISOTOPICALLY LABELED COMPOUNDS

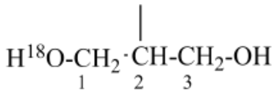
P-46.2.1 The principal substituent chain contains the greater number of isotopically modified atoms.

Examples:



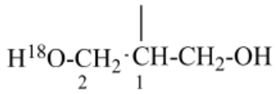
$$\overset{4}{C}H_2[^2H]\text{-}\underset{3}{\overset{CH_3}{C}}H\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}H_2\text{—}$$

(1) 3-methyl[4-$^2H_1$]butyl (preferred prefix)



$$H^{18}O\text{-}\underset{1}{C}H_2\text{-}\underset{2}{\overset{|}{C}}H\text{-}\underset{3}{C}H_2\text{-}OH$$

(2)



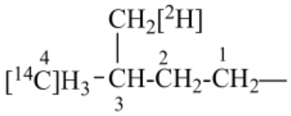
$$H^{18}O\text{-}\underset{2}{C}H_2\text{-}\underset{1}{\overset{|}{C}}H\text{-}CH_2\text{-}OH$$

(1)

(2) 1-(^{18}O)hydroxy-3-hydroxypropan-2-yl (preferred prefix)
(1) 2-(^{18}O)hydroxy-1-(hydroxymethyl)ethyl

P-46.2.2 The principal substituent chain contains the greater number of nuclides of higher mass number or isotopically modified substituent atoms or groups.

Example:



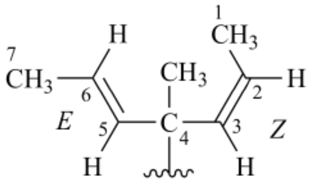
$$[^{14}\overset{4}{C}]H_3\text{-}\underset{3}{\overset{CH_2[^2H]}{C}}H\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}H_2\text{—}$$

(1) 3-[$^2H_1$]methyl[4-^{14}C]butyl (preferred prefix)

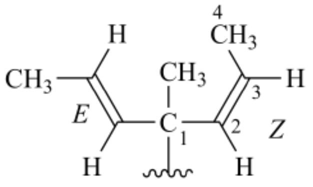
P-46.3 PRINCIPAL SUBSTITUENT CHAINS IN COMPOUNDS WITH STEREOGENIC CENTERS

P-46.3.1 The principal substituent chain contains the greater number of (*Z*)-double bonds.

Examples:



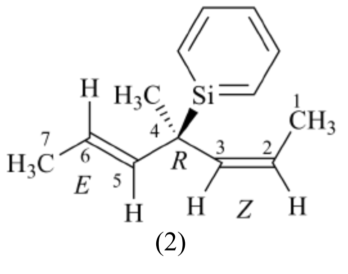
(2)



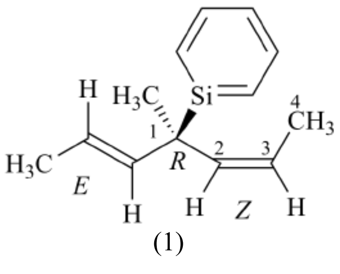
(1)

(2) (2*Z*,5*E*)-4-methylhepta-2,5-dien-4-yl (preferred prefix)
(1) (2*Z*)-1-[(1*E*)-prop-1-en-1-yl]-1-methylbut-2-en-1-yl

Note: The configuration at C-4 (method 2) or C-1 (method 1) cannot be given because the attached substituent is unknown. In the following example, the substitution to the parent hydride ‘siline’ creates a chiral center at C-4 (method 2) or C-1 (method 1) and a ‘*R*’ configuration at these positions.



(2)

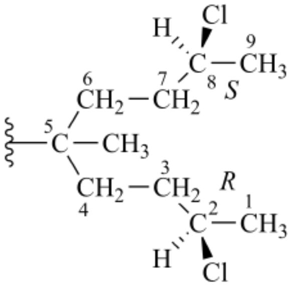


(1)

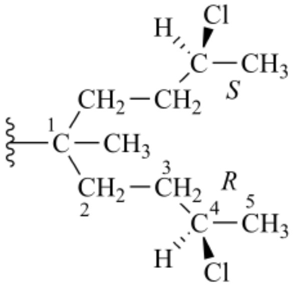
(2) [(2*Z*,4*R*,5*E*)-4-methylhepta-2,5-dien-4-yl]siline (PIN)
(1) {(1*R*,2*Z*)-1-[(1*E*)-prop-1-en-1-yl]-1-methylbut-2-en-1-yl}siline

P-46.3.2 The principal substituent chain contains the greater number of (*R*)-chirality centers.

Examples:


H
Cl
9
C−CH3
7
8
6
S
CH2−CH2
5
C−CH3
3
CH2−CH2
R
4
2
1
C−CH3
H
Cl

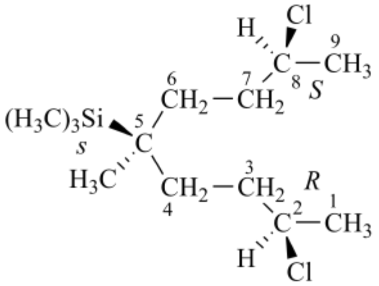
(2)


H
Cl
C−CH3
CH2−CH2
S
1
C−CH3
3
CH2−CH2
R
2
4
5
C−CH3
H
Cl

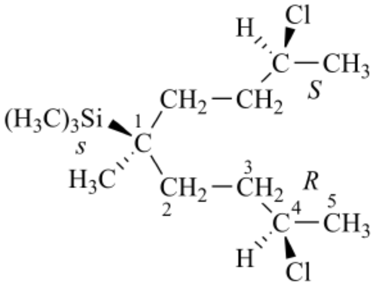
(1)

(2) (2*R*,8*S*)-2,8-dichloro-5-methylnonan-5-yl (preferred prefix)
(1) (4*R*)-4-chloro-1-[(3*S*)-3-chlorobutyl]-1-methylpentyl

Note: The configuration at C-5 (method 2) or C-1 (method 1) cannot be given because the attached substituent is unknown. In the following example, the substitution into the structure 'trimethylsilane' creates a chirality center at C-5 (method 2) or C-1 (method 1) and an '*s*' configuration at these positions.


H
Cl
9
C−CH3
7
8
6
S
CH2−CH2
(H3C)3Si
5
s
C
H3C
3
CH2−CH2
R
4
2
1
C−CH3
H
Cl

(2)


H
Cl
C−CH3
CH2−CH2
S
(H3C)3Si
1
s
C
H3C
3
CH2−CH2
R
2
4
5
C−CH3
H
Cl

(1)

(2) [(2*R*,5*s*,8*S*)-2,8-dichloro-5-methylnonan-5-yl]trimethylsilane (PIN)
(1) {(1*s*,4*R*)-4-chloro-1-[(3*S*)-3-chlorobutyl]-1-methylpentyl}trimethylsilane

Nomenclature of Organic Chemistry. IUPAC Recommendations and Preferred Names 2013.

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Chapter P-5 SELECTING PREFERRED IUPAC NAMES AND CONSTRUCTING NAMES OF ORGANIC COMPOUNDS

P-50 Introduction
P-51 Selecting the preferred type of IUPAC nomenclature
P-52 Selecting preferred IUPAC names and preselected names for parent hydrides
P-53 Selecting preferred retained names of parent hydrides
P-54 Selecting the preferred method for modifying the degree of hydrogenation
P-55 Selecting the preferred retained name for functional parent compounds
P-56 Selecting the preferred suffix for the principal characteristic groups
P-57 Selecting preferred and preselected prefixes for substituent group names
P-58 Selection of preferred IUPAC names
P-59 Name construction

P-50 INTRODUCTION

Many compounds can have two or more names in accordance with several methods recommended by IUPAC for their formation, one of which is recommended herein as the preferred IUPAC name (PIN). This Chapter summarizes the selection rules that are recommended in Chapters P-1 through P-4 for generation of preferred IUPAC names for compounds described in these Chapters and also in Chapters P-6 to P-10 where applicable. Substitutive nomenclature is the principal type of nomenclature for organic compounds; however, other types are recommended because substitutive nomenclature was never recommended for naming certain classes of compounds or because they represent a simplification when the substitutive names become long and cumbersome.

In Chapter P-1, several types of nomenclature are discussed. All of them are used to generate preferred IUPAC names and names for general nomenclature. Functional class nomenclature (see P-51.2) is used to generate names of well defined classes, such as acid halides and esters. Multiplicative nomenclature (see P-51.3) is used to enable several occurrences of the same parent structure in a single molecule all to be expressed as parent structures, although this is permitted only under certain restrictive conditions. When these conditions are not fulfilled, substitutive nomenclature is recommended. Skeletal replacement (‘a’) nomenclature (see P-51.4) is used to simplify substitutive names of acyclic compounds containing heteroatoms (usually by eliminating many nesting operations); it is mandatory for naming saturated heterocyclic compounds having more than ten members and in heteropolyalicyclic nonfused bridged and spiro ring systems.

In Chapter P-2, most of the rules are unequivocal because they generate preferred IUPAC names of cyclic and acyclic compounds in themselves. When rings, ring systems, and chains are composed of entities that are themselves rings or ring systems, interconnected or not by chains, phane nomenclature is recommended to generate preferred IUPAC names; the selection of these names is discussed in P-52.2.5. The selection of preferred IUPAC names for ring assemblies is treated in P-52.2.7. The selection of preferred IUPAC names is also necessary for substituent groups derived from the parent hydrides described in Chapter P-2.

In Chapter P-3, the level of saturation expressed by the prefixes ‘hydro/dehydro’ or ‘ene/yne’ endings is considered. In the cases of characteristic groups cited as prefixes and functional parent compounds, the selection is between retained names and systematic names as components of preferred IUPAC names.

In Chapter P-4, the various seniority orders described are unequivocal, with the exception of substituted parent structures that must be analyzed as preferred IUPAC names. In P-44, comprehensive rules for the selection of a preferred parent structure are presented. A new concept for IUPAC nomenclature is described in Section P-45 called ‘Selection of preferred IUPAC names’. The selection of a preferred IUPAC name is based on hierarchical rules based on seniority orders for determining the one and only preferred parent name based on the senior parent structure described in P-44. This issue is discussed in P-58.

P-51 SELECTING THE PREFERRED IUPAC TYPE OF NOMENCLATURE

P.51.0 Introduction
P-51.1 Selecting the preferred type of nomenclature
P-51.2 Functional class nomenclature (see P-15.2)
P-51.3 Multiplicative nomenclature (see P-15.3)
P-51.4 Skeletal replacement (‘a’) nomenclature (see P-15.4)
P-51.5 Conjunctive nomenclature *vs.* substitutive nomenclature

P-51.0 INTRODUCTION

When a choice is needed between the several types of IUPAC nomenclature, the following selection rules must be applied. Sections P-51.1 through P-51.4 give specific rules for each type of nomenclature and examples.

P-51.1 SELECTING THE PREFERRED TYPE OF NOMENCLATURE

When there is a choice between two types of nomenclature, the preferred type of nomenclature is selected in accordance with the following rules.

P-51.1.1 Substitutive nomenclature is preferred to functional class nomenclature, except for the classes described in P-51.2 for which no substitutive names are prescribed.

Example:

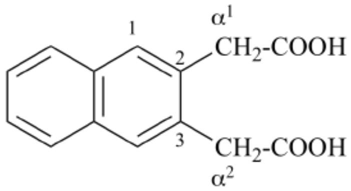
$(CH_3)_2C{=}N{-}N{=}C(CH_3)_2$

acetone azine (see P-68.3.1.2.3)

di(propan-2-ylidene)hydrazine (PIN)

P-51.1.2 Substitutive nomenclature is preferred to conjunctive nomenclature.

Example:



2,3-naphthalenediacetic acid (a conjunctive name)

2,2′-(naphthalene-2,3-diyl)diacetic acid (PIN; a substitutive name; see P-15.6.1.4)

P-51.1.3 Skeletal replacement ('a') nomenclature is preferred to substitutive nomenclature when heteroatoms are present in chains (see P-51.4.1) and the criteria for the use of skeletal nomenclature are met.

Example:

$$\overset{8}{CH_3}\text{-}\overset{7}{SiH_2}\text{-}\overset{6}{CH_2}\text{-}\overset{5}{SiH_2}\text{-}\overset{4}{CH_2}\text{-}\overset{3}{PH}\text{-}\overset{2}{SiH_2}\text{-}\overset{1}{CH_3}$$

3-phospha-2,5,7-trisilaoctane (PIN, a skeletal replacement ('a') name)

(methylsilyl)({[(methylsilyl)methyl]silyl}methyl)phosphane (a substitutive name)

P-51.1.4 Skeletal replacement ('a') nomenclature is preferred to multiplicative nomenclature (see P-51.4.1) when the criteria for use of skeletal nomenclature are met.

Example:

$$\overset{1}{CH_3}\text{-}\overset{2}{SiH_2}\text{-}\overset{3}{CH_2}\text{-}\overset{4}{SiH_2}\text{-}\overset{5}{CH_2}\text{-}\overset{6}{SiH_2}\text{-}\overset{7}{CH_2}\text{-}\overset{8}{S}\text{-}\overset{9}{CH_2}\text{-}\overset{10}{CH_3}$$

8-thia-2,4,6-trisiladecane (PIN, skeletal replacement ('a') name)

1-[(ethylsulfanyl)methyl]-1′-methyl-1,1′-[silanediylbis(methylene)]bis(silane); (a multiplicative name)

P-51.1.5 Multiplicative nomenclature (P-15.3, P-51.3), as a subset of substitutive nomenclature, is preferred to simple substitutive nomenclature when the criteria for its use are met; it allows multiple occurrences of the principal characteristic group or compound class to be treated together.

Example:

$$HOOC\text{-}\overset{2}{CH_2}\text{-}O\text{-}CH_2\text{-}CH_2\text{-}O\text{-}\overset{2'}{CH_2}\text{-}COOH$$

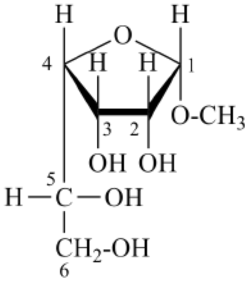
2,2′-[ethane-1,2-diylbis(oxy)]diacetic acid (PIN, multiplicative name)

[2-(carboxymethoxy)ethoxy]acetic acid (substitutive name)

P-51.2 FUNCTIONAL CLASS NOMENCLATURE

In many cases, functional class nomenclature and substitutive nomenclature can be used to give two names to one compound, for example methyl bromide, a functional class name, and bromomethane, a substitutive name, for CH_3-Br. Substitutive names have now replaced many functional class names, but not all. In the context of preferred IUPAC names, it is essential to correctly use the two types of nomenclature. In P-51.2.1, the functional class names that are preferred IUPAC names are given. In P-51.2.2 the functional class names that may be used in general nomenclature are discussed and exemplified; for the substitutive names that are the preferred IUPAC names corresponding to these functional class names, see P-15.2.

P-51.2.1 Functional class nomenclature is used to generate preferred IUPAC names for the following characteristic groups.

Amine oxides	$(CH_3)_3NO$ *N*,*N*-dimethylmethanamine *N*-oxide (PIN; P-62.5) (trimethylazaniumyl)oxidanide (*N*,*N*-dimethylmethanaminiumyl)oxidanide
Imine oxides	$CH_2{=}N(O)Cl$ *N*-chloromethanimine *N*-oxide (PIN; P-62.5) [chloro(methylidene)azaniumyl]oxidanide (*N*-chloromethaniminiumyl)oxidanide
Acyl halides	$CH_3\text{-}CO\text{-}Cl$ acetyl chloride (PIN; P-65.5.1)
Acyl azides	$CH_3\text{-}CH_2\text{-}CH_2\text{-}CO\text{-}N_3$ butanoyl azide (PIN; P-65.5.2.1)
Acyl cyanides	$CH_3\text{-}CH_2\text{-}CO\text{-}CN$ propanoyl cyanide (PIN; P-65.5.2.1)
Acyl isocyanides	$C_6H_5\text{-}CO\text{-}NC$ benzoyl isocyanide (PIN; P-65.5.2.1)
Acyl isocyanates (same for S, Se, Te)	$CH_3\text{-}CO\text{-}NCO$ acetyl isocyanate (PIN; P-65.5.2.1
Esters	$CH_3\text{-}CO\text{-}O\text{-}CH_3$ methyl acetate (PIN; P-65.6.3.2.1)
Anhydrides	$CH_3\text{-}CO\text{-}O\text{-}CO\text{-}CH_2\text{-}CH_3$ acetic propanoic anhydride (PIN; P-65.7.2)
Acid halides, pseudohalides [derived from class 7(c) acids]	$CH_3\text{-}N(O)Cl_2$ methylazonic dichloride (PIN; P-67.1.2.5)
Acid amides [derived from class7(d) acids]	$CH_3\text{-}NH\text{-}SO\text{-}NH_2$ *N*-methylsulfurous diamide (PIN; P-67.1.2.6)
Acid hydrazides [derived from class 7(c) acids]	$(CH_3)_2P\text{-}NH\text{-}NH_2$ dimethylphosphinous hydrazide (PIN; P-67.1.2.6)
Glycosides	 H O H 4 H H 1 O-CH₃ 3 2 OH OH 5 H—C—OH CH₂-OH 6 methyl α-D-gulofuranoside (P-102.5.6.2.2)

P-51.2.2 Functional class nomenclature for general nomenclature

A certain number of classes can still be named for general nomenclature by applying functional class nomenclature. They are described in P-15.2. For these classes, preferred IUPAC names are substitutive names.

Examples:

$CH_3\text{-}CH_2\text{-}CN$	ethyl cyanide propanenitrile (PIN)

C_6H_5-NC	phenyl isocyanide isocyanobenzene (PIN)
$(CH_3)_2C$=N-N=$C(CH_3)_2$	acetone azine (see P-68.3.1.2.3) di(propan-2-ylidene)hydrazine (PIN)
CH_3-CH_2-CH=N-OH	propanal oxime *N*-propylidenehydroxylamine *N*-hydroxypropan-1-imine (PIN)
$(CH_3)_2C$=N-NH-CO-NH_2	acetone semicarbazone 2-(propan-2-ylidene)hydrazinecarboxamide (PIN)

P-51.3 MULTIPLICATIVE NOMENCLATURE (see P-15.3)

Multiplicative nomenclature is used to name assemblies of identical units linked by di- or polyvalent groups formed according to P-15.3.2. This subsection describes the formation of preferred IUPAC multiplicative names according to the principles and rules discussed in P-15.3. Substitutive nomenclature is used when the conditions for constructing multiplicative names are not met. Further, skeletal replacement (‘a’) nomenclature (see P-15.4) and phane nomenclature (see P-26) are used rather than multiplicative nomenclature when the conditions for their use are met in order to simplify name construction when multiplicative names become complex and cumbersome.

In these recommendations, identical parent structures do not have to have a principal characteristic group in order to construct a multiplicative name, which was necessary in earlier recommendations.

P-51.3.1 Preferred IUPAC multiplicative names

For a multiplicative name to be categorized as an IUPAC preferred name, certain restrictive conditions must be met. Multiplicative nomenclature is preferred to substitutive nomenclature for generating preferred IUPAC names to express multiple occurrences of identical parent structures, other than alkanes when

(1) the linking bonds (single or multiple) between the central substituent group of the multiplicative group and all subsequent structural units are identical and

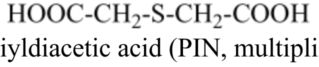
(2) the multiplicative groups, other than the central multiplicative group, are symmetrically substituted; and

(3) the locants of all substituent groups on the identical parent structures, including suffix groups, are identical.

In these recommendations, all substituent groups, including the principal characteristic groups must be identical and have the same locant in order to construct a multiplicative name. This is a change from earlier recommendations where such locants did not need to be identical.

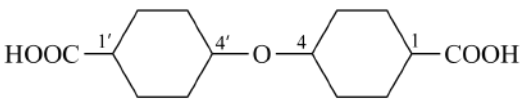
The first two specific conditions are related to the linking di- or polyvalent groups. They are defined and exemplified in Section P-15.3.1.2. Simple and concatenated groups are used when the conditions expressed in P-15.3.1.2.1 and P-15.3.1.2.2 are fulfilled.

Examples:

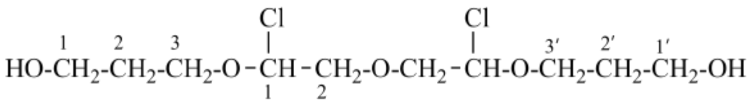


$\text{HOOC-}\overset{2}{\text{C}}\text{H}_2\text{-S-}\overset{2'}{\text{C}}\text{H}_2\text{-COOH}$

2,2′-sulfanediyldiacetic acid (PIN, multiplicative name)
[(carboxymethyl)sulfanyl]acetic acid (substitutive name)

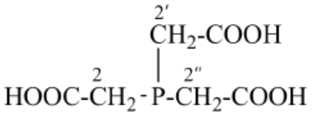


4,4′-oxydi(cyclohexane-1-carboxylic acid) (PIN, multiplicative name)
4-[(4-carboxycyclohexyl)oxy]cyclohexane-1-carboxylic acid (substitutive name)



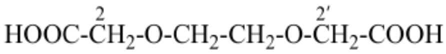
$\text{HO-}\overset{1}{\text{C}}\text{H}_2\text{-}\overset{2}{\text{C}}\text{H}_2\text{-}\overset{3}{\text{C}}\text{H}_2\text{-O-}\underset{1}{\overset{\text{Cl}}{\text{CH}}}\text{-}\underset{2}{\text{CH}_2}\text{-O-CH}_2\text{-}\overset{\text{Cl}}{\text{CH}}\text{-O-}\overset{3'}{\text{C}}\text{H}_2\text{-}\overset{2'}{\text{C}}\text{H}_2\text{-}\overset{1'}{\text{C}}\text{H}_2\text{-OH}$

3,3′-{oxybis[(1-chloroethane-2,1-diyl)]oxy}di(propan-1-ol) (PIN,
a multiplicative name)
3-{2-[2-chloro-2-(3-hydroxypropoxy)ethoxy]-1-chloroethoxy}propan-1-ol
(a substitutive name)



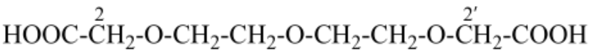
$$\mathrm{HOOC\text{-}\overset{2}{C}H_2\text{-}\underset{}{P}(\overset{2'}{C}H_2\text{-}COOH)\text{-}\overset{2''}{C}H_2\text{-}COOH}$$

2,2′,2″-phosphanetriyltriacetic acid (PIN, a multiplicative name)
[bis(carboxymethyl)phosphanyl]acetic acid (a substitutive name)



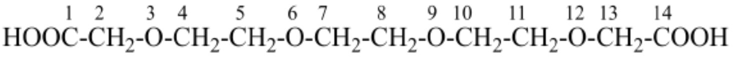
$$\mathrm{HOOC\text{-}\overset{2}{C}H_2\text{-}O\text{-}CH_2\text{-}CH_2\text{-}O\text{-}\overset{2'}{C}H_2\text{-}COOH}$$

2,2′-[ethane-1,2-diylbis(oxy)]diacetic acid (PIN, a multiplicative name)
[2-(carboxymethoxy)ethoxy]acetic acid (a substitutive name)



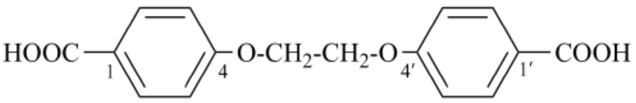
$$\mathrm{HOOC\text{-}\overset{2}{C}H_2\text{-}O\text{-}CH_2\text{-}CH_2\text{-}O\text{-}CH_2\text{-}CH_2\text{-}O\text{-}\overset{2'}{C}H_2\text{-}COOH}$$

2,2′-[oxybis(ethane-2,1-diyloxy)]diacetic acid (PIN, a multiplicative name)
{2-[2-(carboxymethoxy)ethoxy]ethoxy}acetic acid (a substitutive name)

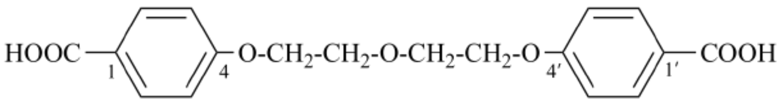


$$\mathrm{HOO\overset{1}{C}\text{-}\overset{2}{C}H_2\text{-}\overset{3}{O}\text{-}\overset{4}{C}H_2\text{-}\overset{5}{C}H_2\text{-}\overset{6}{O}\text{-}\overset{7}{C}H_2\text{-}\overset{8}{C}H_2\text{-}\overset{9}{O}\text{-}\overset{10}{C}H_2\text{-}\overset{11}{C}H_2\text{-}\overset{12}{O}\text{-}\overset{13}{C}H_2\text{-}\overset{14}{C}OOH}$$

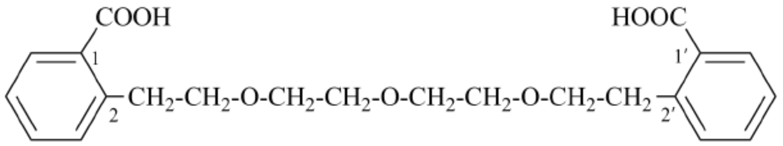
3,6,9,12-tetraoxatetradecane-1,14-dioic acid [PIN,
a skeletal replacement (‘a’) name]
2,2′-[ethane-1,2-diylbis(oxyethane-2,1-diyloxy)]diacetic acid
(a multiplicative name)
(2-{2-[2-(carboxymethoxy)ethoxy]ethoxy}ethoxy)acetic acid (a substitutive name)



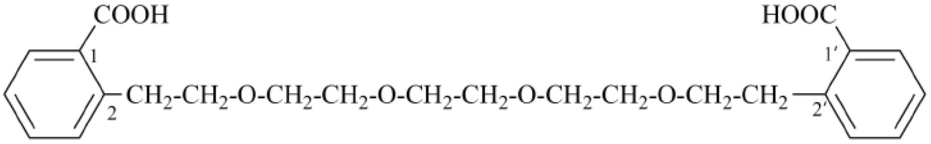
4,4′-[ethane-1,2-diylbis(oxy)]dibenzoic acid (PIN, a multiplicative name)
4-[2-(4-carboxyphenoxy)ethoxy]benzoic acid (a substitutive name)



4,4′-[oxybis(ethane-2,1-diyloxy)]dibenzoic acid (PIN, a multiplicative name)
4-{2-[2-(4-carboxyphenoxy)ethoxy]ethoxy}benzoic acid (a substitutive name)



2,2′-[oxybis(ethane-2,1-diyloxyethane-2,1-diyl)]dibenzoic acid (PIN,
a multiplicative name)
2-[2-(2-{2-[2-(2-carboxyphenyl)ethoxy]ethoxy}ethoxy)ethyl]benzoic acid
(a substitutive name)

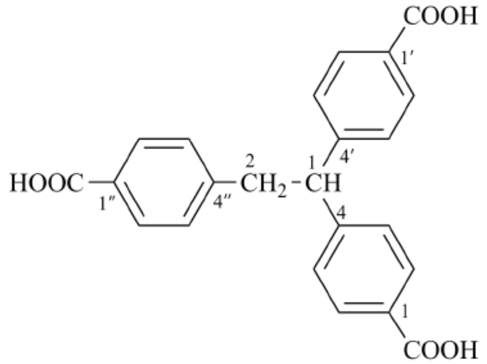


2,2′-(3,6,9,12-tetraoxatetradecane-1,14-diyl)dibenzoic acid (PIN,
a multiplicative name using the skeletal replacement (‘a’) name as the multiplying substituent group)
2,2′-[ethane-1,2-diylbis(oxyethane-2,1-diyloxyethane-2,1-diyl)]dibenzoic acid
(a multiplicative name using simple substitutive nomenclature)
2-{2-[2-(2-{2-[2-(2-carboxyphenyl)ethoxy]ethoxy}ethoxy)ethoxy]ethyl}benzoic acid (a substitutive name)

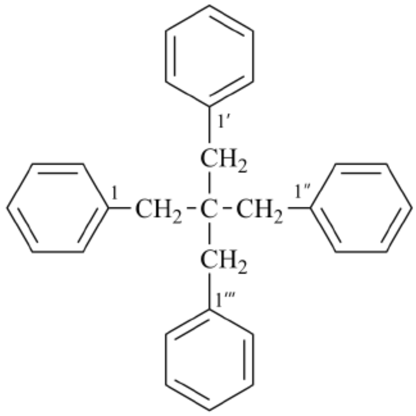
P-51.3.2 When more than two identical parent structures occur in the structure, the following rules are to be followed in choosing preferred IUPAC names. Note that preferred IUPAC names are formed using phane nomenclature when four or more rings are present, two being terminal, in a system containing a minimum of seven nodes [see P-52.2.5.1 (2)] and skeletal replacement (‘a’) nomenclature is used when the conditions for its use are met (see P-15.4.3, P-44.4, and P-51.4).

P-51.3.2.1 A maximum number of identical parent structures must be expressed by the multiplicative name.

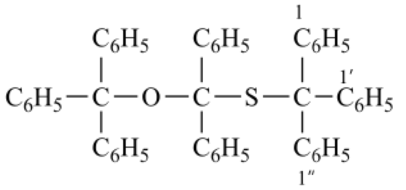
Examples:



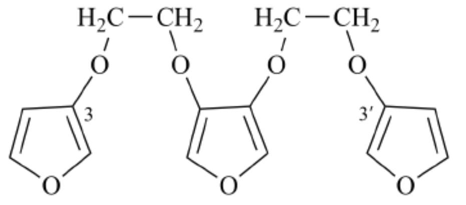
4,4′,4″-(ethane-1,1,2-triyl)tribenzoic acid (PIN)
[not 4,4″-[2-(4-carboxyphenyl)ethane-1,1-diyl]dibenzoic acid;
the preferred IUPAC name multiplies more identical parent structures ‘3’ *vs.* ‘2’; see P-15.3.3.2.1]



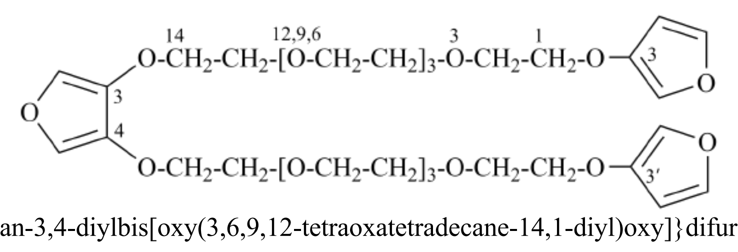
1,1′-(2,2-dibenzylpropane-1,3-diyl)dibenzene (PIN, a multiplicative name;
a multiplicative prefix name such as neopentanetetrayl has never been recognized)
(2,2-dibenzyl-3-phenylpropyl)benzene (substitutive name)



1,1′,1″-({[diphenyl(triphenylmethoxy)methyl]sulfanyl}methanetriyl)tribenzene (PIN)
[not 1,1′-{(triphenylmethoxy)[(triphenylmethyl)sulfanyl]methylene}dibenzene];
this name multiplies only two identical parent structures]
[not 1,1′,1″-({diphenyl[(triphenylmethyl)sulfanyl]methoxy}methanetriyl)tribenzene;
the PIN is lower alphabetically
(‘diphenyltriphenylmethoxy’ is lower alphabetically than ‘diphenyltriphenylmethyl’)]



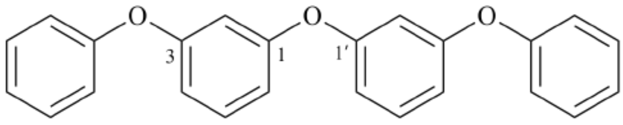
3,3′-[furan-3,4-diylbis(oxyethane-2,1-diyloxy)]difuran (PIN, a multiplicative name)
3,4-bis[2-(furan-3-yloxy)ethoxy]furan (a substitutive name)]



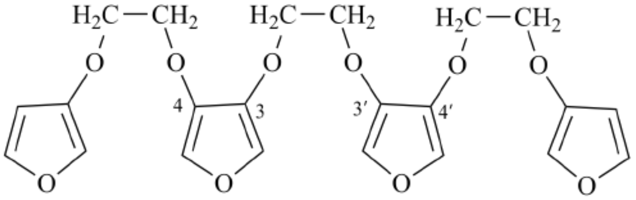
3,3′-{furan-3,4-diylbis[oxy(3,6,9,12-tetraoxatetradecane-14,1-diyl)oxy]}difuran (PIN)

P-51.3.2.2 When the parent structure occurs more than three times and not all the occurrences are connected to a single multiplicative substituent group, the identical units to be multiplied are those nearer to the central unit of the multiplicative substituent group; the other parent structures are expressed as substituents to the multiplicative name. Preferred IUPAC names are formed by skeletal replacement (‘a’) nomenclature or phane nomenclature when the conditions for use of these methods are met [see P-51.4 and P-52.2.5.1, respectively].

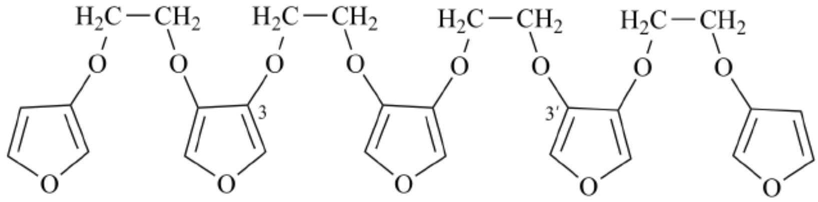
Examples:



1,1′-[oxybis(3,1-phenyleneoxy)dibenzene (a multiplicative name)
2,4,6-trioxa-1,7(1),3,5(1,3)-tetrabenzenaheptaphane (PIN, a phane name, see P-51.4, P-52.2.5)



3,3′-[ethane-1,2-diylbis(oxy)]bis{4-[2-(furan-3-yloxy)ethoxy]furan} (a multiplicative name)
[not 3,3′-[ethane-1,2-diylbis(oxyfuran-4,3-diyloxyethane-2,1-diyloxy)]difuran (a multiplicative name)]
2,5,7,10,12,15-hexaoxa-1,16(3),6,11(3,4)-tetrafuranahexadecaphane (PIN; a phane name, see P-51.4, P-52.2.5)



3,3′-[furan-3,4-diylbis(oxyethane-2,1-diyloxy)]bis{4-[2-(furan-3-yloxy)ethoxy]furan}
(a multiplicative name)
[not 3,4-bis[2-({4-[2-(furan-3-yloxy)ethoxy]furan-3-yl}oxy)ethoxy]furan (a substitutive name)]
[not 3,3′-[furan-3,4-diylbis(oxyethane-2,1-diyloxyfuran-4,3-diyloxyethane-2,1-diyloxy)]difuran (a multiplicative name)]
2,5,7,10,12,15,17,20-octaoxa-1,21(3), 6,11,16(3,4)-pentafuranahenicosaphane (PIN,
a phane name, see P-51.4, P-52.2.5)

P-51.3.2.3 Seniority order of classes (see P-41) is used when a choice has to be made between a parent structure and a component of a multiplicative group.

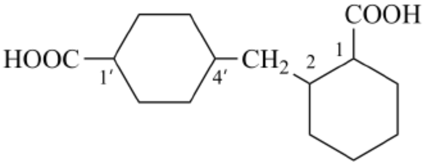
Example:

$$C_6H_5\text{-}\overset{2}{N}{=}\overset{1}{N}\text{-}CO\text{-}\overset{1'}{N}{=}N\text{-}C_6H_5$$

bis(phenyldiazenyl)methanone (PIN)
[not 1,1′-carbonylbis(2-phenyldiazene);
not 1,1′-[carbonylbis(diazenediyl)]dibenzene;
methanone is senior to both ‘diazene’ and a carbocyclic ring, see P-41]

P-51.3.3 When conditions (1), (2), and (3) as defined in P-51.3.1, above, are not met, the preferred IUPAC name is generated by substitutive nomenclature principles.

Examples:



2,4′-methylenedi(cyclohexane-1-carboxylic acid) (a multiplicative name)
2-[(4-carboxycyclohexyl)methyl]cyclohexane-1-carboxylic acid (PIN,
a substitutive name, see P-45.2.2)
[not 4-[(2-carboxycyclohexyl)methyl]cyclohexane-1-carboxylic acid;
the substituent locant ‘2’ is lower than ‘4’ (see P-14.3.5, P-45.2.2)]
$H_3Si\text{-}SiH_2\text{-}CH_2\text{-}OO\text{-}SiH_2\text{-}SiH_3$
[(disilanylmethyl)peroxy]disilane (PIN, a substitutive name)
[not [(disilanylperoxy)methyl]disilane;
‘disilanylmethylperoxy’ precedes ‘disilanylperoxymethyl’ in alphanumerical order (see P-45.5)]

More examples are found in P-15.3, and in P-44, P-45, and P-46.

P-51.4 SKELETAL REPLACEMENT (‘a’) NOMENCLATURE

Skeletal replacement (‘a’) nomenclature is used to generate preferred IUPAC names in place of substitutive or multiplicative names when four or more heterounits are present in an acyclic chain (see P-51.3.1). Skeletal replacement (‘a’) nomenclature is the only recommended method for certain types of cyclic compounds.

> In these recommendations, groups of atoms having a simple multivalent name are considered as a unit, hence the term heterounits includes both heteroatoms and heterogroups. Heterogroups were not considered as a single heterounit in previous recommendations.

P-51.4.1 Skeletal replacement (‘a’) nomenclature in acyclic chains

P-51.4.1.1 Skeletal replacement (‘a’) nomenclature rather than substitutive or multiplicative names must be used to generate preferred IUPAC names for acyclic structures when four or more heterounits are present in a unbranched chain containing at least one carbon atom and when none of the heteroatoms constitute all or part of the principal characteristic group of the compound.

A heterounit is a set of heteroatoms having a name of its own such as, –SS–, disulfanediyl; $–SiH_2\text{-}O\text{-}SiH_2–$, disiloxane-1,3-diyl; –SOS–, dithioxanediyl (not $–OSiH_2O–$ nor –OSO– that correspond to three consecutive units ‘oxysilanediyloxy’ and ‘oxysulfanediyloxy’, respectively). Acids such as carbonic acid or phosphorus, arsenic, and antimony acids, when representing the parent compound or the principal group, are not considered as units. In presence of a characteristic group having seniority for citation as a suffix, the group $–O\text{-}P(O)(OCH_3)\text{-}O–$ is composed of three units (see example 11 below).

P-51.4.1.2 Skeletal replacement (‘a’) nomenclature generates new acyclic parent hydrides whose numbering is fixed, as it is for heterocyclic rings and ring systems. Suffixes, endings, and prefixes are added in accordance with this fixed numbering.

> Fixed numbering for heteroacyclic parent structures named by skeletal replacement (‘a’) nomenclature is a major change to Rule C-0.6 (ref. 1) where principal characteristic groups and free valence were preferred over heteroatoms for low locants.

Examples:

$$\overset{8}{CH_3}\text{-}\overset{7}{SiH_2}\text{-}\overset{6}{CH_2}\text{-}\overset{5}{SiH_2}\text{-}\overset{4}{CH_2}\text{-}\overset{3}{PH}\text{-}\overset{2}{SiH_2}\text{-}\overset{1}{CH_3}$$

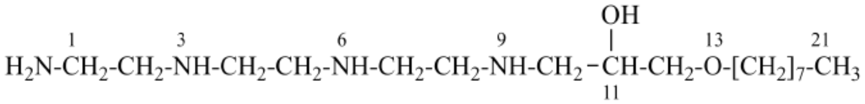
3-phospha-2,5,7-trisilaoctane [PIN, skeletal replacement (‘a’) name]
(methylsilyl)({[(methylsilyl)methyl]silyl}methyl)phosphane (a substitutive name)

$$\overset{1}{CH_3}\text{-}\overset{2}{SiH_2}\text{-}\overset{3}{CH_2}\text{-}\overset{4}{SiH_2}\text{-}CH_2\text{-}\overset{6}{SiH_2}\text{-}\overset{7}{CH_2}\text{-}\overset{8}{S}\text{-}\overset{9}{CH_2}\text{-}\overset{10}{CH_3}$$

8-thia-2,4,6-trisiladecane [PIN, skeletal replacement (‘a’) name]
1-[(ethylsulfanyl)methyl]-1′-methyl-1,1′-[silanediylbis(methylene)]bis(silane); (a multiplicative name)
({[(ethylsulfanyl)methyl]silyl}methyl)[(methylsilyl)methyl]silane; (a substitutive name)

$$HOO\overset{1}{C}\text{-}\overset{2}{CH_2}\text{-}\overset{3}{O}\text{-}\overset{4}{CH_2}\text{-}\overset{5}{CH_2}\text{-}\overset{6}{O}\text{-}\overset{7}{CH_2}\text{-}\overset{8}{CH_2}\text{-}\overset{9}{O}\text{-}\overset{10}{CH_2}\text{-}\overset{11}{CH_2}\text{-}\overset{12}{O}\text{-}\overset{13}{CH_2}\text{-}\overset{14}{COOH}$$

3,6,9,12-tetraoxatetradecanedioic acid [PIN, a skeletal replacement (‘a’) name]
2,2′-{ethane-1,2-diylbis[(oxyethane-2,1-diyl)oxy]diacetic acid; (a multiplicative name)
2-(2-{2-[2-(carboxymethoxy)ethoxy]ethoxy}ethoxy)acetic acid; (a substitutive name)

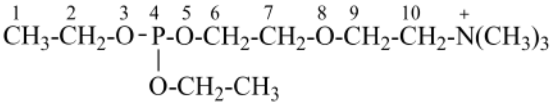


$$H_2N\text{-}\overset{1}{CH_2}\text{-}CH_2\text{-}\overset{3}{NH}\text{-}CH_2\text{-}CH_2\text{-}\overset{6}{NH}\text{-}CH_2\text{-}CH_2\text{-}\overset{9}{NH}\text{-}CH_2-\overset{OH}{\underset{11}{CH}}\text{-}CH_2\text{-}\overset{13}{O}\text{-}[CH_2]_7\text{-}\overset{21}{CH_3}$$

1-amino-13-oxa-3,6,9-triazahenicosan-11-ol [PIN; a skeletal replacement (‘a’) name]
1-{[2-({2-[(2-aminoethyl)amino]ethyl}amino)ethyl]amino}-3-(octyloxy)propan-2-ol; (a substitutive name)

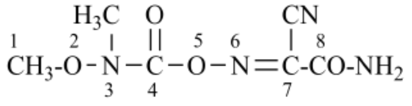
$$F\text{-}\overset{1}{CO}\text{-}\overset{2}{NH}\text{-}\overset{3}{S}\text{-}\overset{4}{NH}\text{-}\overset{5}{CH_2}\text{-}\overset{6}{O}\text{-}\overset{7}{N}=\overset{8}{CH}\text{-}\overset{9}{CH}=\overset{10}{N}\text{-}\overset{11}{O}\text{-}\overset{12}{CH_2}\text{-}\overset{13}{NH}\text{-}\overset{14}{S}\text{-}\overset{15}{NH}\text{-}\overset{16}{CO}\text{-}F$$

6,11-dioxa-3,14-dithia-2,4,7,10,13,15-hexaazahexadeca-7,9-dienedioyl difluoride (PIN)
(a skeletal replacement name)
(an acyclic dioyl fluoride is preferred to a multiplied carbamoyl fluoride)



$$\overset{1}{CH_3}\text{-}\overset{2}{CH_2}\text{-}\overset{3}{O}-\underset{O\text{-}CH_2\text{-}CH_3}{\overset{4}{P}}\text{-}\overset{5}{O}\text{-}\overset{6}{CH_2}\text{-}\overset{7}{CH_2}\text{-}\overset{8}{O}\text{-}\overset{9}{CH_2}\text{-}\overset{10}{CH_2}\text{-}\overset{+}{N}(CH_3)_3$$

4-ethoxy-*N*,*N*,*N*-trimethyl-3,5,8-trioxa-4-phosphadecan-10-aminium (PIN)



$$\overset{1}{CH_3}\text{-}\overset{2}{O}-\overset{H_3C}{\underset{3}{N}}-\overset{O}{\underset{4}{\overset{\|}{C}}}-\overset{5}{O}-\overset{6}{N}=\overset{CN}{\underset{7}{C}}\text{-}\overset{8}{CO}\text{-}NH_2$$

7-cyano-3-methyl-4-oxo-2,5-dioxa-3,6-diazaoct-6-en-8-amide (PIN)

$\text{CH}_3\text{-}\overset{3}{\text{S}}\text{-S-}\overset{1}{\text{S}}\text{-CH}_2\text{-CH}_2\text{-}\overset{1'}{\text{S}}\text{-S-S-CH}_3$

1,1′-(ethane-1,2-diyl)bis(3-methyltrisulfane) (PIN)
(not 2,3,4,7,8,9-hexathiadecane; trisulfane, HS-S-SH, is
a parent hydride and is not allowed to be a heterounit)

$(\text{CH}_3)_3\text{C-OO-Si(CH}_3)_2\text{-O-CO-CH}_2\text{-CH}_3$

(*tert*-butylperoxy)dimethylsilyl propanoate (PIN)
(not 2,2,5,5-tetramethyl-3,4,6-trioxa-5-silanonan-7-one;
only two heterounits are present: –OO– and –Si–;
the principal characteristic group is an ester and the –O– is a part of it)

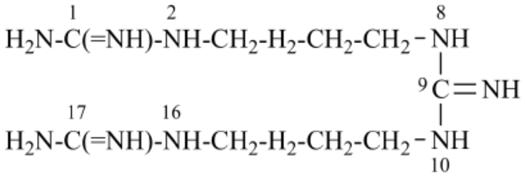
$\text{CH}_3\text{-O-PH(O)-O-CH}_2\text{-O-CH}_3$

methoxymethyl methyl phosphonate (PIN)
[not 2,4,6-trioxa-3λ^5-phosphaheptan-3-one;
the three heteroatoms –O-P-O– are part of an ester and are expressed
as the principal characteristic group; this leaves only one heterounit, –O–,
and skeletal replacement (‘a’) nomenclature cannot be used as the PIN]

$\text{CH}_3\text{-O-P(O)(OCH}_3\text{)-O-}\overset{1}{\text{C}}\text{H}_2\text{-}\overset{2}{\text{Si}}\text{H}_2\text{-}\overset{3}{\text{C}}\text{H}_2\text{-}\overset{4}{\text{Si}}\text{H}_2\text{-}\overset{5}{\text{C}}\text{H}_2\text{-}\overset{6}{\text{Si}}\text{H}_2\text{-}\overset{7}{\text{C}}\text{H}_2\text{-}\overset{8}{\text{Si}}\text{H}_2\text{-}\overset{9}{\text{C}}\text{H}_3$

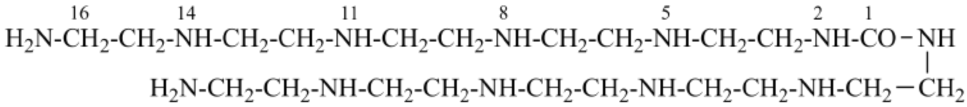
dimethyl 2,4,6,8-tetrasilanonan-1-yl phosphate (PIN)
[three of the heteroatoms –O-P-O– are part of the ester expressed as the principal characteristic group;
however there are four silicon atoms in one of the organyl parts of the ester
and skeletal replacement (‘a’) nomenclature is used to name this ester group]

P-51.4.1.3 The same number of characteristic groups that would be expressed as suffixes in substitutive names must be present in skeletal replacement (‘a’) names.
Examples:



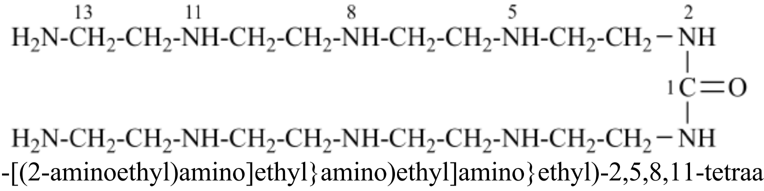
$$\begin{array}{r}
\text{H}_2\text{N-}\overset{1}{\text{C}}\text{(=NH)-}\overset{2}{\text{N}}\text{H-CH}_2\text{-H}_2\text{-CH}_2\text{-CH}_2\text{-}\overset{8}{\text{N}}\text{H}\;\;\;\;\;\;\\
|\;\;\;\;\;\;\;\;\;\;\\
{}^{9}\text{C=NH}\\
|\;\;\;\;\;\;\;\;\;\;\\
\text{H}_2\text{N-}\overset{17}{\text{C}}\text{(=NH)-}\overset{16}{\text{N}}\text{H-CH}_2\text{-H}_2\text{-CH}_2\text{-CH}_2\text{-}\underset{10}{\text{N}}\text{H}\;\;\;\;\;\;
\end{array}$$

9-imino-2,8,10,16-tetraazaheptadecanediimidamide (PIN)
(a diimidamide expressed as a principal characteristic group is senior to a carbonimidic diamide)



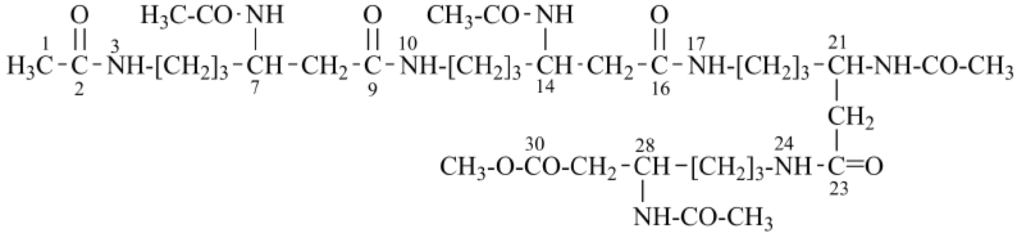
$$\begin{array}{r}
\text{H}_2\overset{16}{\text{N}}\text{-CH}_2\text{-CH}_2\text{-}\overset{14}{\text{N}}\text{H-CH}_2\text{-CH}_2\text{-}\overset{11}{\text{N}}\text{H-CH}_2\text{-CH}_2\text{-}\overset{8}{\text{N}}\text{H-CH}_2\text{-CH}_2\text{-}\overset{5}{\text{N}}\text{H-CH}_2\text{-CH}_2\text{-}\overset{2}{\text{N}}\text{H-}\overset{1}{\text{C}}\text{O-NH}\\
|\;\;\;\\
\text{H}_2\text{N-CH}_2\text{-CH}_2\text{-NH-CH}_2\text{-CH}_2\text{-NH-CH}_2\text{-CH}_2\text{-NH-CH}_2\text{-CH}_2\text{-NH-CH}_2\text{-CH}_2
\end{array}$$

16-amino-*N*-(14-amino-3,6,9,12-tetraazatetradecan-1-yl)-2,5,8,11,14-pentaazahexadecanamide [PIN;
an amide expressed as a principal characteristic group is senior to
urea, a carbonic diamide, or an amine expressed as a principal characteristic group;
since four heteroatoms are also present in the *N*-substituent group,
it must also be named by skeletal replacement (‘a’) nomenclature]



$$\begin{array}{r}
\text{H}_2\overset{13}{\text{N}}\text{-CH}_2\text{-CH}_2\text{-}\overset{11}{\text{N}}\text{H-CH}_2\text{-CH}_2\text{-}\overset{8}{\text{N}}\text{H-CH}_2\text{-CH}_2\text{-}\overset{5}{\text{N}}\text{H-CH}_2\text{-CH}_2\text{-}\overset{2}{\text{N}}\text{H}\;\;\;\\
|\;\;\;\;\;\;\;\\
{}^{1}\text{C=O}\\
|\;\;\;\;\;\;\;\\
\text{H}_2\text{N-CH}_2\text{-CH}_2\text{-NH-CH}_2\text{-CH}_2\text{-NH-CH}_2\text{-CH}_2\text{-NH-CH}_2\text{-CH}_2\text{-NH}\;\;\;
\end{array}$$

13-amino-*N*-(2-{[2-({2-[(2-aminoethyl)amino]ethyl}amino)ethyl]amino}ethyl)-2,5,8,11-tetraazatridecanamide (PIN;
an amide expressed as characteristic group is senior to urea, a carbonic diamide,
and to an amine expressed as a characteristic group;
since only three heteroatoms are present in the *N*-substituent group, it must be named substitutively)



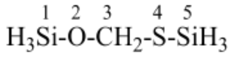
$$\begin{array}{l}
\overset{1}{\text{H}_3\text{C}}\text{-}\underset{2}{\overset{\text{O}\,||}{\text{C}}}\text{-}\overset{3}{\text{N}}\text{H-[CH}_2]_3\text{-}\underset{7}{\overset{\text{H}_3\text{C-CO}\cdot\text{NH}\,|}{\text{CH}}}\text{-CH}_2\text{-}\underset{9}{\overset{\text{O}\,||}{\text{C}}}\text{-}\overset{10}{\text{N}}\text{H-[CH}_2]_3\text{-}\underset{14}{\overset{\text{CH}_3\text{-CO-NH}\,|}{\text{CH}}}\text{-CH}_2\text{-}\underset{16}{\overset{\text{O}\,||}{\text{C}}}\text{-}\overset{17}{\text{N}}\text{H-[CH}_2]_3\text{-}\overset{21}{\text{C}}\text{H-NH-CO-CH}_3\\
\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad |\\
\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\quad \text{CH}_2\\
\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad |\\
\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad \text{CH}_3\text{-O-}\overset{30}{\text{C}}\text{O-CH}_2\text{-}\underset{\text{NH-CO-CH}_3}{\underset{|}{\overset{28}{\text{C}}\text{H}}}\text{-[CH}_2]_3\text{-}\overset{24}{\text{N}}\text{H-}\underset{23}{\text{C}}\text{=O}
\end{array}$$

methyl 7,14,21,28-tetraacetamido-2,9,16,23-tetraoxo-3,10,17,24-tetraazatriacontan-30-oate (PIN;
an ester is senior to an amide or a ketone)

P-51.4.1.4 The chain must be terminated by C or one of the following heteroatoms: P, As, Sb, Bi, Si, Ge, Sn, Pb, B, Al, Ga, In, or Tl.

In these recommendations heterochains may be terminated by certain heteroatoms and not just by carbon atoms. Previous recommendations required a heterochain to be terminated by carbon atoms.

Example:



$\overset{1}{H_3Si}\text{-}\overset{2}{O}\text{-}\overset{3}{CH_2}\text{-}\overset{4}{S}\text{-}\overset{5}{SiH_3}$

2-oxa-4-thia-1,5-disilapentane (PIN)

P-51.4.2 Skeletal replacement ('a') nomenclature for cyclic compounds

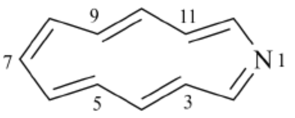
Skeletal replacement ('a') nomenclature is the only recommended method to generate names for certain heterocyclic compounds.

P-51.4.2.1 Skeletal replacement ('a') nomenclature is used to derive preferred IUPAC names for heteromonocyclic compounds having more than ten ring atoms (see P-22.2.3).

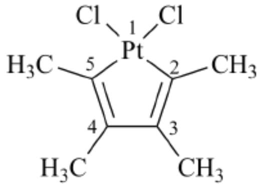
Skeletal replacement ('a') nomenclature is also possible with rings having less than 10 ring members if the skeletal replacement ('a') prefix represents a metal as defined in P-69.4.

Adapting the principles of the Hantzsch-Widman system to the elements of Groups 1-12 in and including their skeletal replacement ('a') prefixes would be a major change from previous recommendations even though the names of such organometallic compounds involving these elements are not PINs at this time.

Examples:



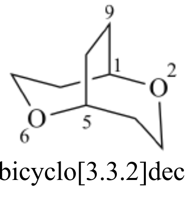
1-azacyclododeca-1,3,5,7,9,11-hexaene (PIN)



1,1-dichloro-2,3,4,5-tetramethylplatinole (Hantzsch-Widman name)
1,1-dichloro-2,3,4,5-tetramethyl-1-platinacyclopenta-2,4-diene
(a skeletal replacement name; see P-69.4)

The option to include the metallic elements in addition to the metals in Groups 13 through 16 in the Hantzsch-Widman system and their skeletal replacement ('a') prefixes (see P-69.4) is a major change from previous recommendations for the Hantzsch-Widman system.

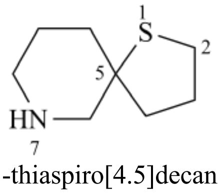
P-51.4.2.2 Skeletal replacement ('a') nomenclature is used to derive preferred IUPAC names for heterocyclic von Baeyer ring systems (see P-23.3.1).
Example:



2,6-dioxabicyclo[3.3.2]decane (PIN)

P-51.4.2.3 Skeletal replacement ('a') nomenclature is used to derive preferred IUPAC names for heterocyclic spiro parent hydrides consisting of two or more saturated monocyclic rings (see P-24.2.4.1.1)

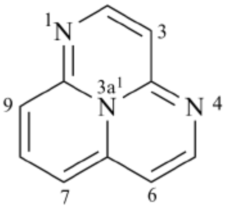
Example:



7-aza-1-thiaspiro[4.5]decane (PIN)

P-51.4.2.4 Skeletal replacement ('a') nomenclature is used to derive preferred IUPAC names for heteropolycyclic ring systems for which fusion nomenclature based on heterocyclic parent rings is not applicable (see P-25.5.1).

Example:

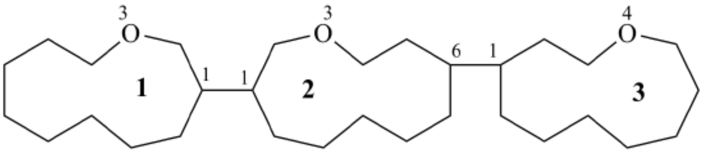


1,3a^1,4-triazaphenylene (PIN)
[not 1,4,9b-triazaphenylene; see P-25.3.3.3]

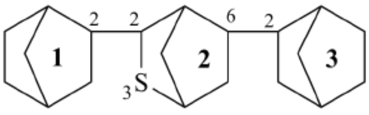
P-51.4.2.5 Skeletal replacement (‘a’) nomenclature is used to derive preferred IUPAC names for heterophane ring systems (see P-26.5) and for heterofullerenes (see P-27.5).

P-51.4.2.6 When necessary, the choice of a preferred IUPAC name of a heterocyclic parent structure is made before the insertion of skeletal replacement (‘a’) prefixes. This is the case with assemblies of identical heterocyclic compounds (see P-28.4) composed of heterocyclic compounds of the von Baeyer type and with monocyclic compounds having more than ten members.

Examples:



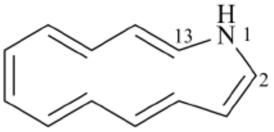
1^3,2^3,3^4-trioxa-1^1,2^1:2^6,3^1-tercycloundecane (PIN; see P-28.3.1)
3,3′,4″-trioxa-1,1′:6′,1″-tercycloundecane
(not 1^3,2^3:2^9,3^4-ter-1-oxacycloundecane)



2^3-thia-1^2,2^2:2^6,3^2-terbicyclo[2.2.1]heptane (PIN; see P-28.3.1)
{not 2,6-bis(bicyclo[2.2.1]heptan-2-yl)-3-thiabicyclo[2.2.1]heptane}
3′-thia-2,2′:6′,2″-terbicyclo[2.2.1]heptane

P-51.4.2.7 The choice between two or more acceptable names may depend on the type of nomenclature used. This is the case with unsaturated heteromonocyclic compounds for which three names are acceptable, as discussed in P-52.2.3.

Example:

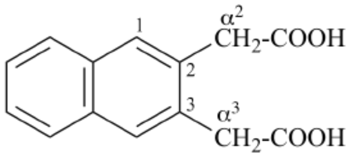


1-azacyclotrideca-2,4,6,8,10,12-hexaene [PIN, a skeletal replacement (‘a’) name]
1-azacyclotridecine [a skeletal relacement (‘a’) name for use in fusion nomenclature]
1*H*-1-aza[13]annulene

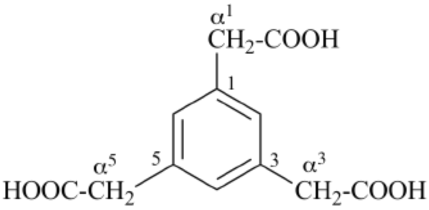
P-51.5 CONJUNCTIVE NOMENCLATURE *vs.* SUBSTITUTIVE NOMENCLATURE

When there is a choice between conjunctive nomenclature and substitutive nomenclature, preferred IUPAC names are formed by using substitutive nomenclature (including multiplicative nomenclature and skeletal replacement nomenclature when the conditions for their use are fulfilled) (see P-51).

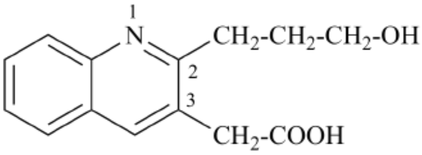
Examples:



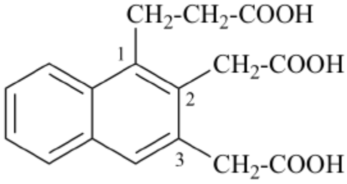
naphthalene-2,3-diacetic acid
2,2′-(naphthalene-2,3-diyl)diacetic acid (PIN)



benzene-1,3,5-triacetic acid
2,2′,2″-(benzene-1,3,5-triyl)triacetic acid (PIN)



2-(3-hydroxypropyl)quinoline-3-acetic acid
[2-(3-hydroxypropyl)quinolin-3-yl]acetic acid (PIN)
(a carboxylic acid is senior to an alcohol)



1-(2-carboxyethyl)naphthalene-2,3-diacetic acid
3-[2,3-bis(carboxymethyl)naphthalen-1-yl]propanoic acid (PIN)

P-52 SELECTING PREFERRED IUPAC NAMES AND PRESELECTED NAMES (see P-12.2) FOR PARENT HYDRIDES

For naming the parent hydrides described in Chapter P-2, when only one method is described, the resulting single names are naturally preferred IUPAC names. When more than one method is recommended for generating the names of parent hydrides, preferred IUPAC names, and in some cases preselected names, must be chosen. Some retained names are used as preferred IUPAC names and as names for use in general nomenclature.

P-52.1 Selecting preselected names
P-52.2 Selecting preferred IUPAC names

P-52.1 SELECTING PRESELECTED NAMES

P-52.1.1 Mononuclear parent hydride names are listed in P-21.1.1. Phosphane, PH_3, arsane, AsH_3, stibane, SbH_3, and bismuthane, BiH_3, are preselected names; the names phosphine, arsine, stibine, and bismuthine, respectively, are retained for use in general nomenclature.

P-52.1.2 Preselected names for homogeneous acyclic polynuclear parent hydrides are described in P-21.2.2. The preselected name for NH_2-NH_2 is the retained name hydrazine; the systematic name diazane may be used in general nomenclature.

P-52.1.3 Preselected names for heterogeneous acyclic parent hydrides composed of alternating ‘ab’ atoms, i.e., [a(ba)$_n$ parent hydrides], except carbon or halogen, are described in P-21.2.3.1.

In these recommendations, the ‘amine’ characteristic group is recognized in a(ba)$_n$ parent hydrides, which is a change from earlier recommendations where it was not recognized. In addition, carbon was not excluded as a ‘b’ element leading to conflicts with the order of priority for heteranes.

Examples:

SnH_3-O-SnH_2-O-SnH_3
tristannoxane (preselected name)
[not bis(stannyloxy)stannane]

CH_3-NH-CH_3
N-methylmethanamine (PIN)
(not dicarbazane)

HSe-S-Se-S-SeH
triselenathiane (preselected name)

$SiH_3\text{-}NH\text{-}SiH_2\text{-}NH\text{-}SiH_3$
N,*N*′-disilylsilanediamine (based on silane, a preselected name)
(not trisilazane)

P-52.1.4 Preselected names for parent hydrides with nonstandard bonding numbers are discussed in P-21.1.2.1.

Examples:

PH_5
λ^5-phosphane (preselected name)
phosphorane

AsH_5
λ^5-arsane (preselected name)
arsorane

SH_4
λ^4-sulfane (preselected name)
(not sulfurane)

SH_6
λ^6-sulfane (preselected name)
(not persulfurane)

IH_3
λ^3-iodane (preselected name)
(not iodinane)

IH_5
λ^5-iodane (preselected name
(not periodinane)

SbH_5
λ^5-stibane (preselected name)
stiborane

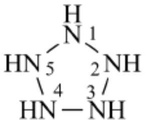
$\overset{1}{\mathrm{SH}}\text{-}\overset{2}{\mathrm{SH_2}}\text{-}\overset{3}{\mathrm{SH}}$
2λ^4-trisulfane (preselected name)

P-52.1.5 Heteromonocyclic noncarbon Hantzsch-Widman parent hydrides

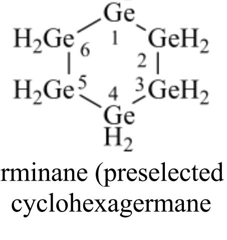
The final ‘e’ in Hantzsch-Widman names is required in preferred IUPAC names; it is still optional in general nomenclature. In the 1979 Rules (ref. 1), the final ‘e’ of a Hantzsch-Widman name was omitted when there was no nitrogen in the ring; in the 1993 Guide (ref. 2) this omission was made optional.

P-52.1.5.1 Preselected names for homogeneous heteromonocyclic parent hydrides consisting of ten or fewer ring members are Hantzsch-Widman names (see P-22.2.2). Skeletal replacement (‘a’) names are preselected names for homogeneous heteromonocyclic parent hydrides with more than ten ring members (see P-22.2.3). Alternative names, which may be used in general nomenclature, are those formed by using the prefix ‘cyclo’ (see P-22.2.5).

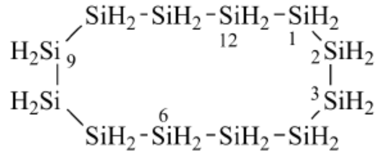
Examples:



pentazolidine (preselected name)
cyclopentaazane



hexagerminane (preselected name)
cyclohexagermane

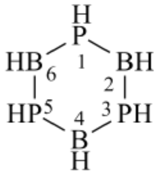


dodecasilacyclododecane (preselected name; see P-12.2)
cyclododecasilane

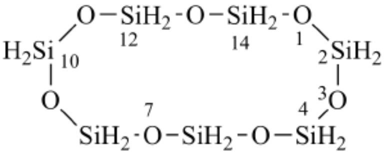
P-52.1.5.2 Heterogeneous heteromonocyclic parent hydrides consisting of alternating heteroatoms

Preselected names for heterogeneous heteromonocyclic parent hydrides with ten or fewer ring members and consisting of alternating heteroatoms, i.e., $[ab]_n$, are Hantzsch-Widman names (see P-22.2.2). Skeletal replacement ('a') names (see P-22.2.3) are preselected names for heterogeneous monoheterocyclic parent hydrides with alternating heteroatoms with more than ten ring members. Alternative names for use only in general nomenclature are those formed by using the prefix 'cyclo' (see P-52.1).

Examples:



1,3,5,2,4,6-triphosphatriborinane (preselected name)
cyclotriboraphosphane

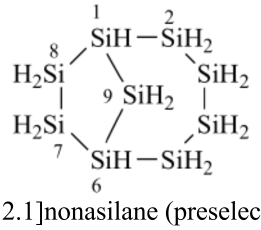


1,3,5,7,9,11,13-heptaoxa-2,4,6,8,10,12,14-heptasilacyclotetradecane (preselected name)
cycloheptasiloxane

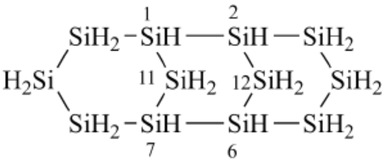
P-52.1.6 Heterocyclic noncarbon von Baeyer and spiro compounds

P-52.1.6.1 Preselected names for von Baeyer compounds and for spiro compounds having only monocyclic components and consisting entirely of heteroatoms of the same kind are names formed by citing the appropriate prefix, such as 'bicyclo', 'spiro', etc., and descriptor enclosed within square brackets followed by a numerical prefix for the total number of heteroatoms and the name of the mononuclear parent hydride; alternative names for use in general nomenclature are formed by skeletal replacement ('a') nomenclature (see P-23.4 and P-24.2.4.2).

Examples:



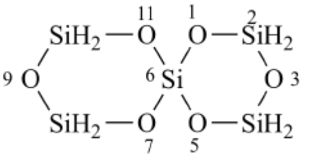
bicyclo[4.2.1]nonasilane (preselected name)
nonasilabicyclo[4.2.1]nonane



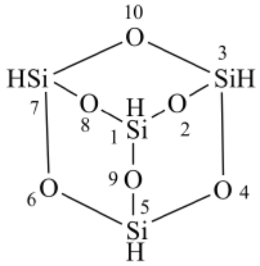
tricyclo[5.3.1.1^{2,6}]dodecasilane (preselected name)
dodecasilatricyclo[5.3.1.1^{2,6}]dodecane

P-52.1.6.2 Preselected names for von Baeyer compounds and for spiro compounds having only monocyclic components and consisting of alternating heteroatoms, i.e., $[ab]_n$, are formed by citing the appropriate prefix, such as 'bicyclo', 'spiro', etc., and a descriptor enclosed within square brackets followed by the number of the ('a') heteroatom, the skeletal replacement name of the ('a') atom, and the skeletal replacement name of the ('b') heteroatom (see P-24.2.4.3); alternative names for use in general nomenclature are those formed by skeletal replacement ('a') nomenclature.

Examples:



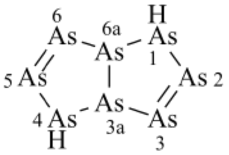
spiro[5.5]pentasiloxane (preselected name)
1,3,5,7,9,11-hexaoxa-2,4,6,8,10-pentasilaspiro[5.5]undecane



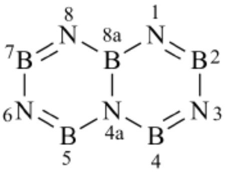
tricyclo[3.3.1.1^{3,7}]tetrasiloxane (preselected name)
2,4,6,8,9,10-hexaoxa-1,3,5,7-tetrasilaadamantane
2,4,6,8,9,10-hexaoxa-1,3,5,7-tetrasilatricyclo[3.3.1.1^{3,7}]decane

P-52.1.7 Preselected names for homogeneous and heterogeneous heterobi- and heteropolycyclic fused ring systems are formed by fusion nomenclature principles (see P-25.3.2.4). Alternative names for use in general nomenclature are formed by prefixing the appropriate 'a' prefixes in front of the name of the hydrocarbon fused ring system.

Examples:



1*H*,4*H*-pentarsolopentarsole (preselected name)
1*H*,4*H*-octaarsapentalene (numbering shown)



[1,3,5,2,4,6]triazatriborinino[1,2-*a*][1,3,5,2,4,6]triazatriborinine (preselected name)
1,3,4a,6,8-pentaaza-2,4,5,7,8a-pentaboranaphthalene (numbering shown)

P-52.2 SELECTING PREFERRED IUPAC NAMES

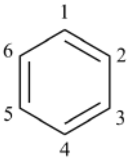
- P-52.2.1 Acyclic and monocyclic hydrocarbons
- P-52.2.2 Heteroacyclic and heteromonocycles
- P-52.2.3 Unsaturated heteromonocyclic compounds with more than ten ring members.
- P-52.2.4 Preferred IUPAC names in fusion nomenclature
- P-52.2.5 Preferred IUPAC names in phane nomenclature
- P-52.2.6 Selecting preferred IUPAC names for (C_{60}-I_h)[5,6]fullerene and (C_{70}-$D5_{h(6)}$)[5,6]fullerene modified by 'nor' or 'seco' prefixes
- P-52.2.7 Preferred IUPAC names and numbering for ring assemblies
- P-52.2.8 Selection between a ring and a chain as parent hydride

P-52.2.1 Acyclic and monocyclic hydrocarbons

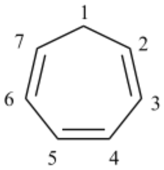
P-52.2.1.1 The names methane, ethane, propane, and butane are used as preferred IUPAC names for CH_4, CH_3-CH_3, CH_3-CH_2-CH_3, and CH_3-CH_2-CH_2-CH_3, respectively. Acetylene is the preferred IUPAC name for $HC{\equiv}CH$ but substitution is not allowed. Limited substitution is allowed in general nomenclature, see P-15.1.8.2.2.

P-52.2.1.2 The name [*n*]annulene is used in preferred IUPAC names as a parent component in fusion nomenclature (see P-25.3.2.1.1) and may be used in general nomenclature as the name for the monocycle itself. Preferred IUPAC names for cycloalkenes and cycloalkapolyenes are generated from the corresponding cycloalkane names (see P-31.1.3.1).

Examples:



benzene (PIN)
(not [6]annulene)



cyclohepta-1,3,5-triene (PIN)
1*H*-[7]annulene (preferred IUPAC name
for the parent component in fusion nomenclature, see P-25.3.2.1.1)

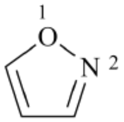
P-52.2.2 Heteroacyclic and heteromonocycles

P-52.2.2.1 Formazan is the preferred IUPAC name retained for HN=N-CH=N-NH$_2$. Hydrazine is the preferred name for H$_2$N-NH$_2$.

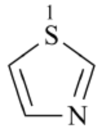
P-52.2.2.2 Preferred IUPAC names for heteromonocyclic rings with no more than ten ring members are Hantzsch-Widman names, including the locants '1,2' and '1,3'. The retained names 'oxazole', 'isoxazole', 'thiazole', and 'isothiazole' are allowed in general nomenclature.

Although the final 'e' in Hantzsch-Widman names is required in preferred IUPAC names; it is still optional in general nomenclature. In the 1979 Rules (ref. 1), the final 'e' of a Hantzsch-Widman name was omitted when there was no nitrogen in the ring; in the 1993 Guide (ref. 2) this omission was made optional.

Examples:



1,2-oxazole (PIN)
isoxazole

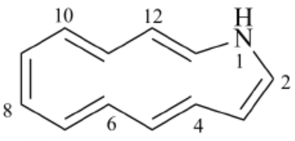


1,3-thiazole (PIN)
thiazole

P-52.2.3 Unsaturated heteromonocyclic compounds with more than ten ring members.

Preferred IUPAC names for unsaturated monocyclic compounds with more than ten ring members derived from cycloalkanes and modified by skeletal replacement ('a') nomenclature are formed by changing the 'ane' ending of the saturated heteromonocycle to 'ene', 'adiene', etc. (see P-31.1.1). [*n*]Annulene names may be used in general nomenclature (see P-31.1.3.2) for the heteromonocycle itself; however, the name 'annulene' cannot be used to designate these heterocyclic compounds as components in fusion nomenclature.

Example:



1-azacyclotrideca-2,4,6,8,10,12-hexaene (PIN)
1-azacyclotridecine [preferred IUPAC name
for the principal component in a fusion name (see also P-25.2.2.1.2)
and 1-azacyclotridecino as an attached component (see P-25.3.2.2.2)]
1*H*-1-aza[13]annulene

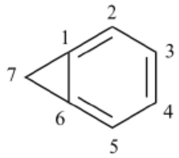
P-52.2.4 Preferred IUPAC names in fusion nomenclature

P-52.2.4.1 Five-membered ring requirement

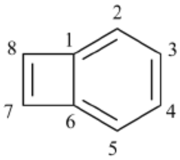
Fusion nomenclature gives preferred IUPAC names only to compounds having at least two rings of at least five or more members. This requirement is not necessarily applied in general nomenclature, in which names such as cyclopropabenzene and cyclobutabenzene can be used. When fusion names are not allowed, unsaturated von Baeyer ring system names are preferred IUPAC names (see P-31.1.4.2).

This is a change from the recommendation in the 1998 publication on fused ring nomenclature (see FR-0, ref. 4) and the 1993 Guide (ref. 2) where no restriction was placed on the size of the two rings that could be used in a fused ring system. For preferred IUPAC names a fusion name can only be used when at least two rings of five or more members are present; this is consistent with recommendations in the 1979 edition (ref. 1). In general nomenclature there is no restriction on the size of rings in a fused ring system.

Examples:



1*H*-cyclopropabenzene
bicyclo[4.1.0]hepta-1,3,5-triene (PIN)

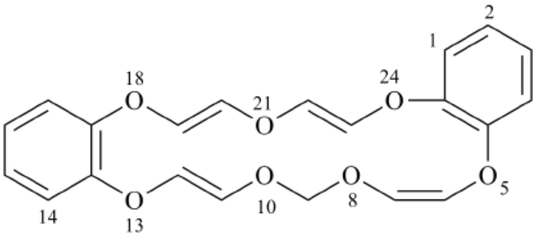


cyclobutabenzene
bicyclo[4.2.0]octa-1,3,5,7-tetraene (PIN)

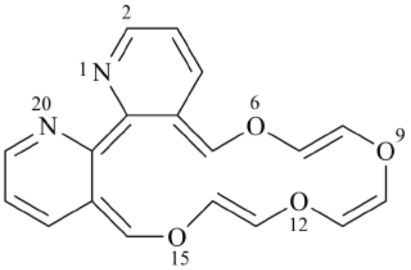
P-52.2.4.2 Heteromonocycles as components in fusion names

Heteromonocycles having more than ten ring members and the maximum number of noncumulative double bonds whose names are denoted by the 'ine' ending described in P-22.2.4 are used as parent components as well as attached components in preferred IUPAC fusion names. 'Annulene' names modified by skeletal replacement ('a') nomenclature (see P-52.2.3) are not recommended for generating names of heterocyclic fusion compounds.

Examples:



9*H*-dibenzo[*g*,*p*][1,3,6,9,12,15,18]heptaoxacycloicosine (PIN; see P-25.3.6.1)

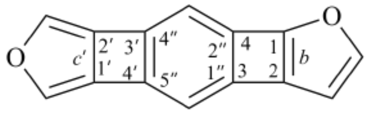


[1,4,7,10]tetraoxacyclohexadecino[13,12-*b*:14,15-*b*′]dipyridine (PIN; see P-25.3.7.1)

P-52.2.4.3 Multiparent fused ring systems with three or more interparent components

When two (or more) possible parent components are separated by an odd number of interparent components and these are ordered symmetrically with respect to their component rings (but not necessarily with their fusion locants), the whole system is treated as a multiparent system. In P-25.3.7.3, second- and higher-order interparent components are named using the multiplying prefixes 'di', 'tri', etc., or 'bis', 'tris', etc. Appropriate locants are assigned to interparent components, unprimed and primed for first-order interparent components, double primed for second-order interparent components, triple primed for third-order interparent components, and so on.

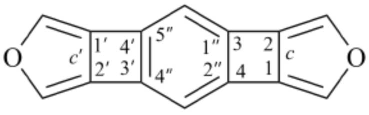
Example:



benzo[1″,2″:3,4;4″,5″:3′,4′]dicyclobuta[1,2-*b*:1′,2′-*c*′]difuran (PIN)

When symmetry permits grouping of interparent components and parent components, such groupings can be formed and cited as such using the prefixes 'bis', 'tris', etc. to denote groups that are enclosed within parentheses. Unprimed locants only are used within such groupings. This method is often encountered and may be used in general nomenclature.

Example:



benzo[1″,2″:3,4;4″,5″,3′,4′]dicyclobuta[1,2-*c*:1′,2′-*c*′]difuran (PIN)
benzo[1″,2″:3,4;4″,5″:3′,4′]bis(cyclobuta[1,2-*c*]furan)

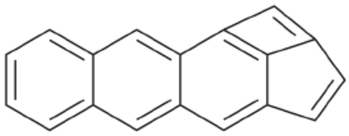
P-52.2.4.4 Limitations to fusion nomenclature

The fusion principles described in P-25.1 through P-25.3 apply to pairs of components. It is not possible by these principles to name a system in which a third component is *ortho*- and *peri*-fused to two components that are themselves *ortho*- or *ortho*- and *peri*-fused together. Hence, when a third component is *ortho*- and *peri*-fused to two components that are themselves *ortho*- or *ortho*- and *peri*-fused together, the following procedures are applied to generate a preferred IUPAC name.

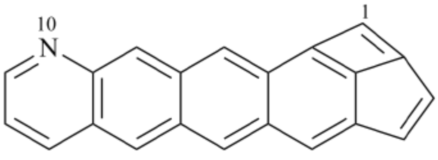
P-52.2.4.4.1 Selection of a less senior parent ring or ring system

P-52.2.4.4.1.1 A less preferred parent ring or ring system component is selected that will permit a fusion name. Second and third choice of parent rings or ring system parent components may be chosen according to the seniority order for selecting the senior ring or ring system as the parent for naming the fused ring system (see P-25.3.2.4).

Examples:



cyclobuta[1,7]indeno[5,6-*b*]naphthalene (PIN)
Explanation: Anthracene cannot be selected as senior parent component; naphthalene, not indene, is next in seniority order for selection as a parent component.

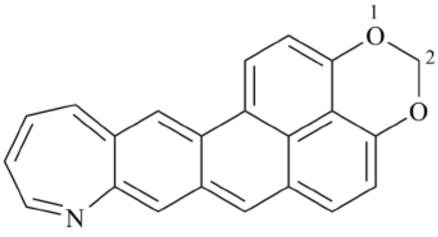


10-azacyclobuta[1,7]indeno[5,6-*b*]anthracene (PIN)

Explanation: Neither quinoline nor pyridine can be used as the senior parent component because neither naphthalene nor anthracene, respectively, can be used as the senior attached component; therefore skeletal replacement ('a') nomenclature must be used (see P-25.5.1); and since the preferred hydrocarbon tetracene cannot be used as the parent hydrocarbon to which skeletal ('a') replacement can be applied (see P-52.2.4.4.2), the next senior component, anthracene, is chosen as the parent hydrocarbon component.

P-52.2.4.4.1.2 It should be noted that benzo heterocycles are considered as one component, thus permitting the construction of fusion names for ring systems that could not otherwise be named by fusion principles.

Example:



2*H*-[1,3]benzodioxino[6′,5′,4′:10,5,6]anthra[2,3-*b*]azepine (PIN)

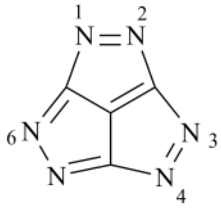
Explanation: A normal fusion name is not possible when the four components azepine, anthracene, 1,3-dioxine, and benzene are treated individually; therefore, the use of a benzo name component is necessary; 1-benzazepine cannot be the parent ring because this would require breaking of the attached component that has a retained name, anthra, which is not allowed, see P-25.3.5.

P-52.2.4.4.2 Skeletal replacement (‘a’) nomenclature

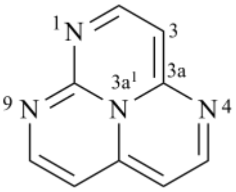
When the fusion principles discussed in P-25.1 through P-25.3 apply, no skeletal replacement (‘a’) name is recommended. This procedure is valid only for cases described here in P-52.2.4.4.2.1.

P-52.2.4.4.2.1 If the corresponding hydrocarbon fused ring system can be named by fusion principles or has a retained name, then heteroatoms are identified by skeletal replacement (‘a’) nomenclature using the appropriate ‘a’ prefixes (see P-22.2.3). The numbering of the fused hydrocarbon system is not altered by the ‘a’ prefixes.

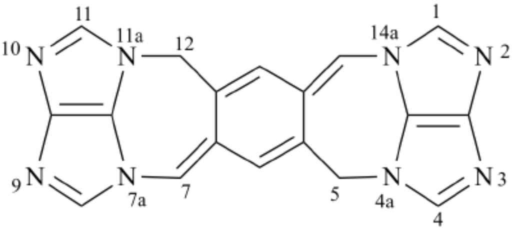
Examples:



1,2,3,4,5,6-hexaazacyclopenta[*cd*]pentalene (PIN)



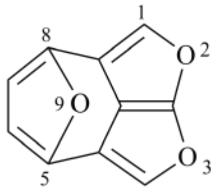
1,3a^1,4,9-tetraazaphenalene (PIN)



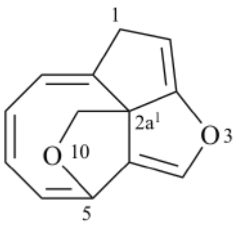
5*H*,12*H*-2,3,4a,7a,9,10,11a,14a-octaazadicyclopenta[*ij*:*i′j′*]benzo[1,2-*f*:4,5-*f′*]diazulene (PIN)

P-52.2.4.4.2.2 If the fused ring system can only be named using skeletal (‘a’) replacement nomenclature, any heteroatoms in bridges are also named using skeletal replacement (‘a’) nomenclature. The replacement terms are cited at the front of the corresponding bridged fused hydrocarbon ring system. Alternatively, the heteroatomic bridge may be named by an appropriate compound or complex bridge prefix.

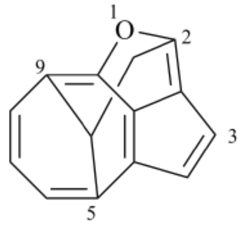
Examples:



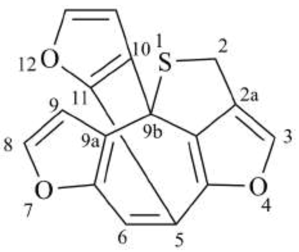
2,3,9-trioxa-5,8-methanocyclopenta[*cd*]azulene (PIN)
5,8-epoxy-2,3-dioxacyclopenta[*cd*]azulene



1*H*-3,10-dioxa-2a^1,5-ethanocycloocta[*cd*]pentalene (PIN)
4*H*-9,2a^1-(epoxymethano)-2-oxacycloocta[*cd*]pentalene



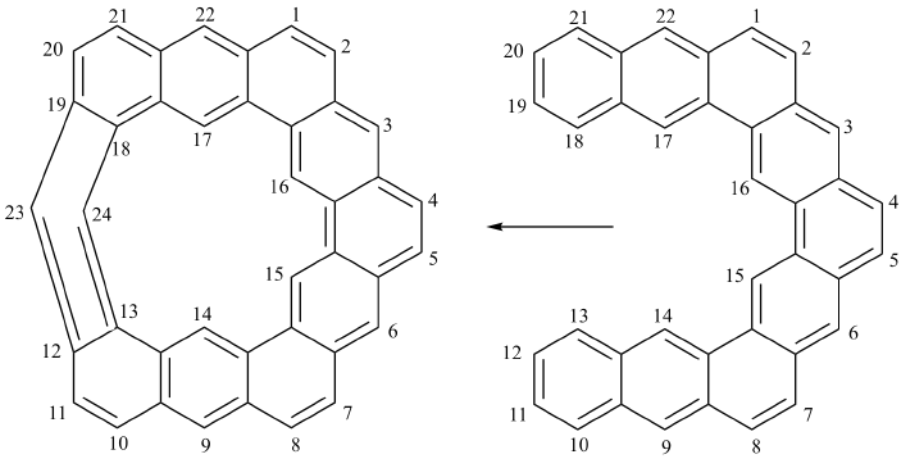
1-oxa-5,9,2-(epiethane[1,1,2]triyl)cycloocta[*cd*]pentalene (PIN)
5,9,2-(epiethane[1,1,2]triyl)-1-oxacycloocta[*cd*]pentalene



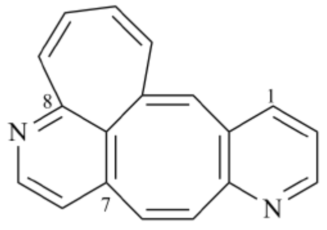
2*H*-4,7,12-trioxa-1-thia-5,9b-[1,2]epicyclopentadicyclopenta[*cd*,*h*]azulene (PIN)
2*H*-5,9b-[2,3]furano-4,7-dioxa-1-thiadicyclopenta[*cd*,*h*]azulene

P-52.2.4.4.3 Bridging nomenclature. A bridged fused system (see Section P-25.4) is used to generate names for structures that cannot be named by normal fusion nomenclature. A properly formed fusion name is first created; then additional rings are created by using bridges.

Examples:



12,19:13,18-di(metheno)dinaphtho[2,3-*a*:2′,3′-*o*]pentaphene (PIN)



8,7-(azenoetheno)cyclohepta[4,5]cycloocta[1,2-*b*]pyridine (PIN)
(not 6,7-buta[1,3]dienocycloocta[1,2-*b*:5,6-*c*′]dipyridine;
the fused ring portion has the maximum number of atoms)

P-52.2.5 Preferred IUPAC names in phane nomenclature

P-52.2.5.1 Cyclic and linear phane structures are described in section P-26. For the purpose of selecting preferred IUPAC names cyclic and acyclic phane systems are defined as follows:

(1) cyclophanes are cyclic phane structures with at least six nodes including two or more rings or ring systems not *ortho* or *ortho* and *peri*-fused to the cyclophane ring, and with at least one ring or ring system of which must be a mancude system;

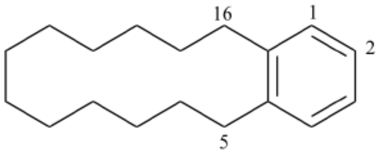
(2) linear phanes consist of four or more rings or ring systems, two of which must be terminal, and together with acyclic atoms or chains must consist of at least seven nodes (components).

P-52.2.5.2 When the conditions given in P-52.2.5.1 for cyclic phane systems are not fulfilled, names of fused ring systems, bridged fused systems, or von Baeyer systems are preferred IUPAC names. The following subsections illustrate these situations.

P-52.2.5.2.1 Mancude systems attached to adjacent atoms of an alicyclic large ring.

Mancude systems attached to adjacent atoms of an alicyclic ring are either fused systems or bridged fused systems. Fusion names described in P-25.0 through P-25.3 or bridged fused ring systems described in P-25.4 are preferred IUPAC names.

Example:

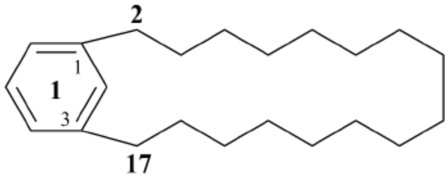


5,6,7,8,9,10,11,12,13,14,15,16-dodecahydrobenzo[14]annulene (PIN)

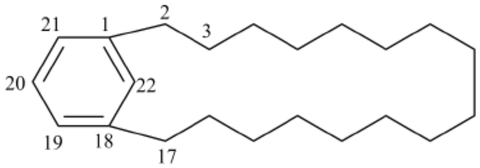
Explanation: A cyclophane name is not allowed.

The seniority order described in P-44.2.2.2 for relevant polycyclic systems is as follows: cyclic phane systems > fused ring systems > bridged fused systems > non-fused bridged systems. The following examples illustrate the application of this seniority order in the derivation of a preferred IUPAC name.

Examples:

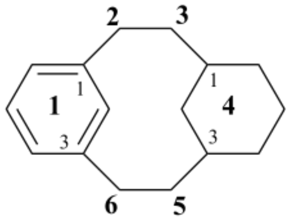


1(1,3)-benzenacycloheptadecaphane
(a phane name)

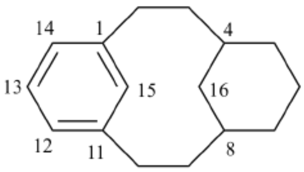


bicyclo[16.3.1]docosa-1(22),18,20-triene
(PIN; a von Baeyer name)

Explanation: Phane name not permitted, only one ring system, see P-52.2.5.1 (1).

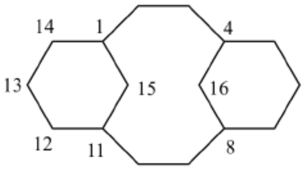


1(1,3)-benzena-4(1,3)-cyclohexanacyclohexaphane (PIN,
a phane name)

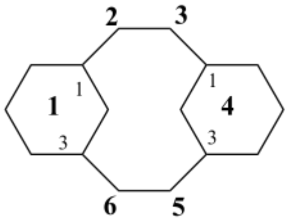


tricyclo[9.3.1.$1^{4,8}$]hexadeca-1(15),11,13-triene
(a von Baeyer name)

Explanation: A fusion name is not possible; a phane name is preferred to a von Baeyer name.

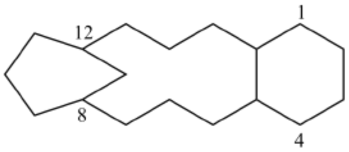


tricyclo[9.3.1.$1^{4,8}$]hexadecane (PIN)
von Baeyer name)

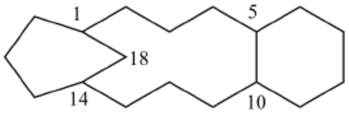


1,4(1,3)-dicyclohexanacyclohexaphane
(phane name)

Explanation: A fusion name is not possible; no mancude ring is present, a phane name is not permitted; therefore the von Baeyer name is the preferred IUPAC name.

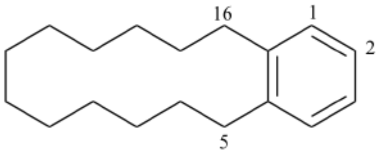


hexadecahydro-1*H*-8,12-methanobenzo[13]annulene (PIN)
(a bridged ring fused name)

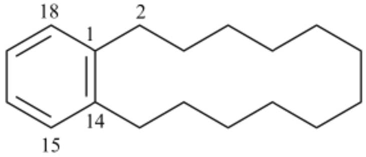


tricyclo[12.3.1.0^{5,10}]octadecane
(a von Baeyer name)

Explanation: No mancude ring, so a phane name is not allowed; the bridged fused ring name is preferred to the von Baeyer name.

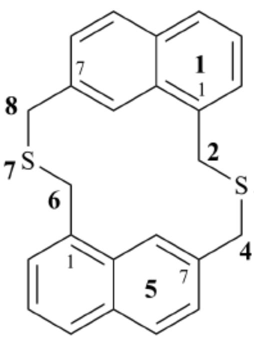


5,6,7,8,9,10,11,12,13,14,15,16-dodecahydrobenzo[14]annulene (PIN)
(fusion name)

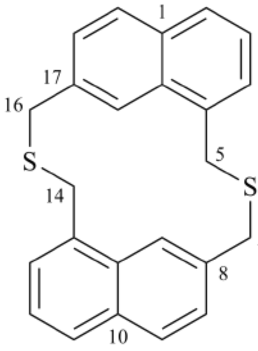


bicyclo[12.4.0]octadeca-1(14),15,17-triene
(von Baeyer name)

Explanation: A phane name not allowed, see Rule P-52.2.5.1; a fusion name is preferred to a von Baeyer name.



(**I**)



(**II**)

(**I**) 3,7-dithia-1(1,7),5(7,1)-dinaphthalenacyclooctaphane (PIN; a phane name)
(**II**) 5,7,14,16-tetrahydro-1,17:8,10-diethenodibenzo[*c*,*j*][1,8]dithiacyclotetradecine
(a bridged fused ring name)

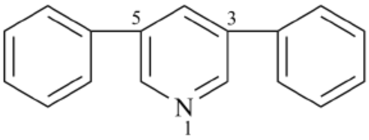
Explanation: A phane name is senior to a bridged fused ring name.

P-52.2.5.3 Ring assemblies, linear phane names, and other linear acyclic/cyclic compounds

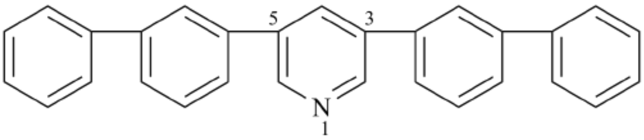
Phane nomenclature is used to generate preferred IUPAC names for ring assemblies and linear acyclic/cyclic compounds that include a minimum of seven nodes including at least four rings or ring systems, two of which must be terminal, even though the compounds could also be named by substitutive or multiplicative nomenclature.

A new numbering system is now recommended for preferred IUPAC names of ring assemblies with more than two rings or ring systems; it consists of composite locants, for example, 1^2. The previous used locant system for ring assemblies with more than two rings or ring systems using serially primed locants (refs. 1 and 2) may be used in general nomenclature.

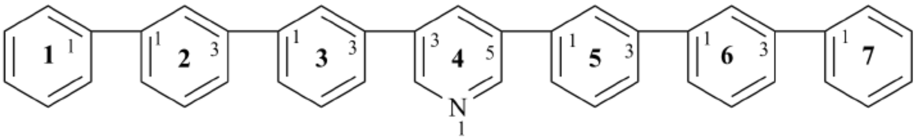
Example 1:



3,5-diphenylpyridine (PIN, substitutive name)

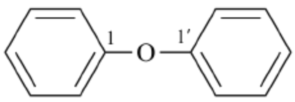


3,5-di([1,1′-biphenyl]-3-yl)pyridine (PIN, substitutive name)

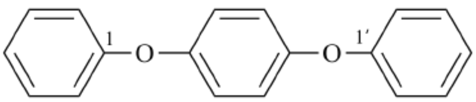


4(3,5)-pyridina-1,7(1),2,3,5,6(1,3)-hexabenzenaheptaphane (PIN, a phane name)
3,5-di([1^1,2^1:2^3,3^1-terphenyl]-1^3-yl)pyridine (a substitutive name, see P-28.3.1)
3,5-di([1,1′:3′,1″-terphenyl]-3-yl)pyridine (a substitutive name)

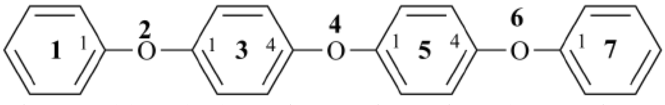
Example 2:



1,1′-oxydibenzene (PIN, a multiplicative name)
phenoxybenzene (a substitutive name)
diphenyl ether (a functional class name)

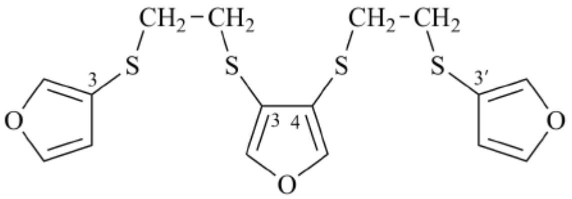


1,1′-[1,4-phenylenebis(oxy)]dibenzene (PIN, a multiplicative name)
1,4-diphenoxybenzene (a substitutive name)

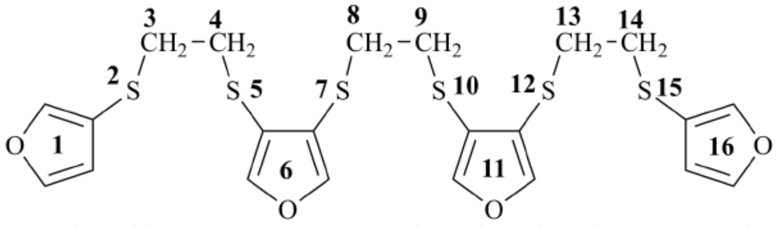


2,4,6-trioxa-1,7(1),3,5(1,4)-tetrabenzenaheptaphane (PIN, a phane name)
1,1′-oxybis(4-phenoxybenzene) (a multiplicative name)
1-phenoxy-4-(4-phenoxyphenoxy)benzene (a substitutive name)

Example 3:



3,3′-[furan-3,4-diylbis(sulfanediylethane-2,1-diylsulfanediyl)]difuran (PIN, multiplicative name)
3,4-bis{[2-(furan-3-ylsulfanyl)ethyl]sulfanyl}furan (substitutive name)



2,5,7,10,12,15-hexathia-1,16(3),6,11(3,4)-tetrafuranahexadecaphane (PIN, a phane name)
3,3′-[ethane-1,2-diylbis(sulfanediyl)]bis(4-{[2-(furan-3-ylsulfanyl)ethyl]sulfanyl}furan) (a multiplicative name)

3-{[2-(furan-3-ylsulfanyl)ethyl]sulfanyl}-4-({2-[(4-{[2-(furan-3-ylsulfanyl)ethyl]sulfanyl}furan-3-yl)sulfany]ethyl}sulfanyl)furan (a substitutive name)

P-52.2.6 Selecting preferred IUPAC names for (C_{60}-I_h)[5,6]fullerene and (C_{70}-$D_{5h(6)}$)[5,6]fullerene modified by ‘nor’ or ‘seco’ prefixes

P-52.2.6.1 Systematic fused and bridged fused ring system names for structures derived from unmodified fullerenes by removal of carbon atoms and rings using a ‘nor operation’, or by removing rings by cutting bonds using a ‘seco’ operation, are often difficult to generate and even more difficult to decipher. Hence, an important objective in naming fullerene fragments is to retain as much as possible of the unmodified fullerene structure on which to base the name. To achieve this, it is recommended that, in order to receive a modified fullerene name, a fullerene fragment must be large enough so as to, arbitrarily, contain more than one-half the number of carbon atoms and more than one-third of the number of rings present in the unmodified fullerene. When these two conditions are fulfilled, a preferred IUPAC name is a modified fullerene name. If at least one of these conditions is not fulfilled the preferred IUPAC name is a fused ring or a bridged fused ring name.

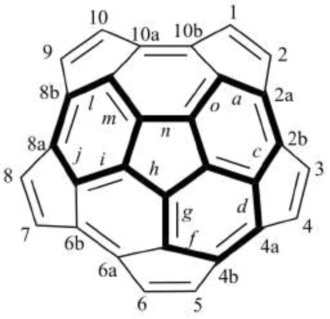
Fragments of a (C_{60}-I_h)[5,6]fullerene or a (C_{70}-$D_{5h(6)}$)[5,6]fullerene derived by removal of carbon atoms or cleavage of bonds are named as norfullerenes, secofullerenes, or seconorfullerenes when **both** of the following two conditions are fulfilled:

(1) the fullerene fragment contains more than one-half of the carbon atoms that were present in the unmodified fullerene, i.e., at least **31 and 36 carbon atoms**, respectively, for the (C_{60}-I_h)[5,6]fullerene and (C_{70}-$D_{5h(6)}$)[5,6]fullerene;

(2) the fullerene fragment must consist of at least one-third of the five- and/or six-membered rings that were present in the unmodified fullerene; i.e., **11 and 13 rings**, respectively, for the (C_{60}-I_h)[5,6]fullerene and (C_{70}-$D_{5h(6)}$)[5,6]fullerene.

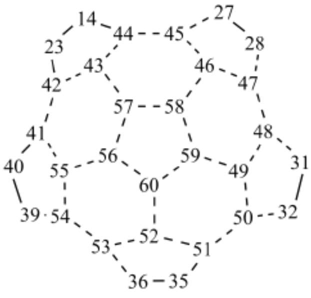
P-52.2.6.2 Nor(C_{60}-I_h)[5,6]fullerenes and nor(C_{70}-$D_{5h(6)}$)[5,6]fullerenes.

Example 1: $C_{30}H_{10}$



10
10a
10b
1
9
2
8b
2a
l
m
o
a
n
8a
2b
j
i
c
8
h
3
g
d
7
f
4
6b
4a
6a
4b
6
5

(**I**)



14
27
23
44
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43
46
42
47
57
58
41
48
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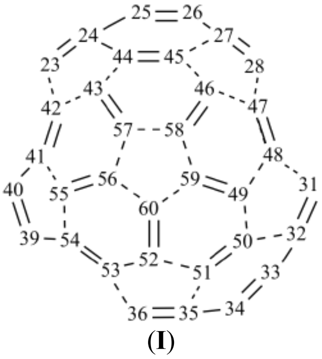
59
40
55
49
31
60
39
54
50
32
53
52
51
36
35

(**II**)

cyclopenta[*cd*]di-*as*-indaceno[3,4,5,6-*fghij*:3′,4′,5′,6′-*lmnoa*]fluoranthene (**I**) (PIN)
[not 1,2,3,4,5,6,7,8,9,10,11,12,13,14,15,16,17,18,19,20,21,22,25,26,29,30,33,34,37,38-triacontanor(C_{60}-I_h)[5,6]fullerene (**II**)]

Explanation: The preferred IUPAC name for this fullerene fragment is a systematic fusion ring name because it contains only 30 carbon atoms.

Example 2: $C_{34}H_{10}$



25
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42
57
58
41
48
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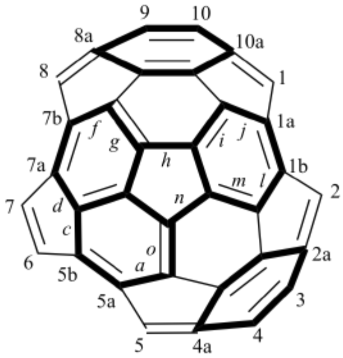
59
49
31
60
39
54
50
32
53
52
51
33
36
35
34

(**I**)



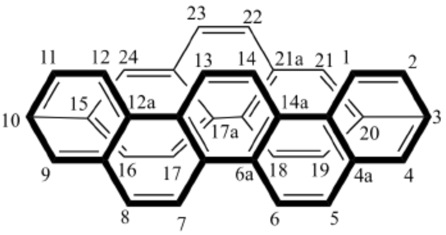
9
10
8a
10a
8
1
7b
1a
f
j
g
i
h
7a
1b
m
l
2
7
d
n
c
6
o
2a
5b
a
3
5a
5
4a
4

(**II**)

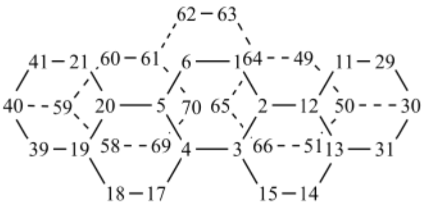
1,2,3,4,5,6,7,8,9,10,11,12,13,14,15,16,17,18,19,20,21,22,29,30,37,38-hexacosanor(C_{60}-I_{h})[5,6]fullerene (**I**) (PIN)
[not bis(benzo[1,8]-*as*-indaceno[3,4,5,6-*fghij*:3′,4′,5′,6′-*lmnoa*])cyclopenta[*cd*]fluoranthene (**II**)]

Explanation: The preferred IUPAC name for this fullerene fragment is a norfullerene name because it contains 34 carbon atoms and 13 rings.

Example 3: $\mathrm{C}_{36}\mathrm{H}_{22}$


23
22
11
12
24
13
14
21a
21
1
2
15
12a
17a
14a
10
20
3
9
16
17
6a
18
19
4a
4
8
7
6
5

(**I**)

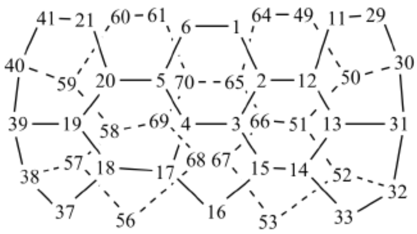

62 − 63
41 − 21
60 − 61
6
164 − − 49
11 − 29
40 − − 59
20
5
70
65
2
12
50 − − − 30
39 − 19
58 − − 69
4
3
66 − − 51
13 − 31
18 − 17
15 − 14

(**II**)

3,10-[2,7]epiphenanthropicene (**I**) (PIN)
[not 7,8,9,10,16,22,23,24,25,26,27,28,32,33,34,35,36,37,38,42,43,44,45,46,47,48,52,53,54,55,56,57,67,68-tetratriacontanor(C_{70}-$D_{5\mathrm{h}(6)}$)[5,6]fullerene (**II**)]

Explanation: The preferred IUPAC name for this fullerene fragment is a systematic bridged fused ring name because it contains only eight rings.

Example 4: $\mathrm{C}_{45}\mathrm{H}_{15}$


41 − 21
60 − 61
6
1
64 − 49
11 − 29
40
59
20
5
70
65
2
12
50
30
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19
58
69
4
3
66
51
13
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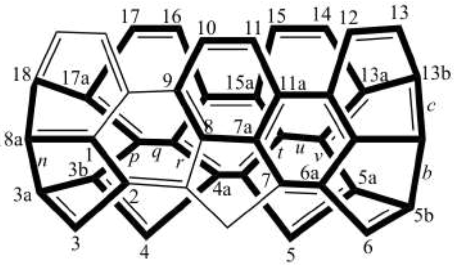
16
53
33

(**I**)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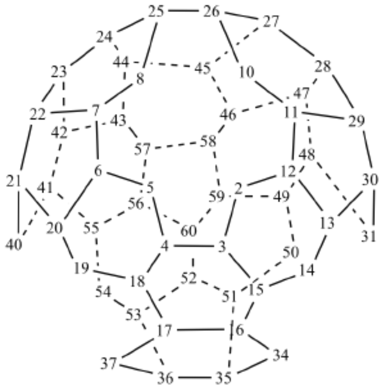
17a
9
15a
11a
13a
13b
c
8
7a
18a
n
1
3b
p
q
r
t
u
v
3a
2
4a
7
6a
5a
b
5b
3
4
5
6

(**II**)

7,8,9,10,22,23,24,25,26,27,28,34,35,36,42,43,44,45,46,47,48,54,55,62,63-pentacosanor(C_{70}-$D_{5\mathrm{h}(6)}$)[5,6]fullerene (**I**) (PIN)
[not 8,7,2-(epiethane[1,2]diyl[1]ylidene)-1,9,18-(epiprop[1]ene[1,1]diyl[3]ylidene)acephenanthryleno[4,3-*bc*]tricyclopenta[*n*,*pqr*,*tuv*]picene (**II**)]

Explanation: The preferred IUPAC name for this fullerene fragment is a norfullerene name because it has 45 carbon atoms and it has 15 rings.

Example 5: $\mathrm{C}_{54}\mathrm{H}_{12}$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58
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6
5
12
30
21
41
56
59
2
49
40
20
55
60
13
31
19
4
3
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54
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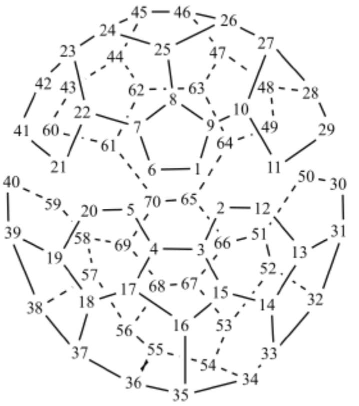
1,9,32,33,38,39-hexanor(C_{60}-I_{h})[5,6]fullerene (PIN)

Explanation: The preferred IUPAC name for this fullerene fragment is a norfullerene name because it has 54 atoms and twenty rings.

P-52.2.6.3 Seco(C_{60}-I_{h})[5,6]fullerenes and seco(C_{70}-$D_{5\mathrm{h}(6)}$)[5,6]fullerenes.

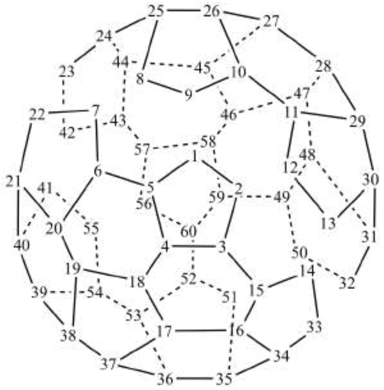
Example 1: $\mathrm{C}_{70}\mathrm{H}_{16}$



1,2:5,6:11,12:20,21:29,30:40,41:49,50:59,60-octaseco(C_{70}-$D_{5h(6)}$)[5,6]fullerene (PIN)

Explanation: The preferred IUPAC name for this fullerene fragment is a secofullerene name because it has 70 carbon atoms and 28 rings.

Example 2: $C_{60}H_{16}$

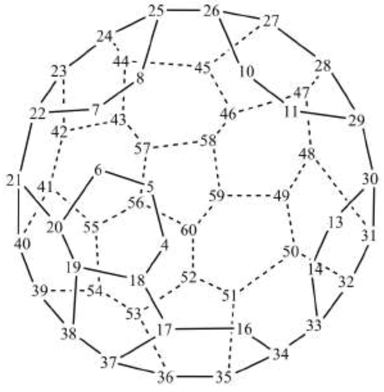


1,9:2,12:7,8:13,14:22,23:32,33:41,42:50,51:55,56-nonaseco(C_{60}-I_h)[5,6]fullerene (PIN)

Explanation: The preferred IUPAC name for this fullerene fragment is a secofullerene name because it has 60 carbon atoms and 21 rings.

P-52.2.6.4. Seconorfullerenes

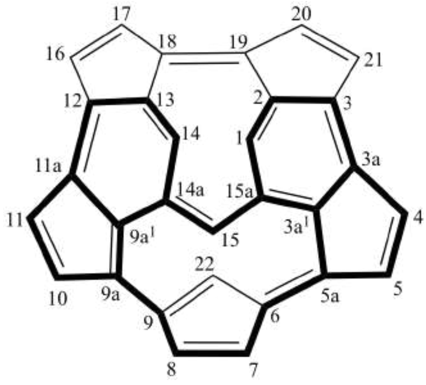
Example 1: $C_{54}H_{10}$



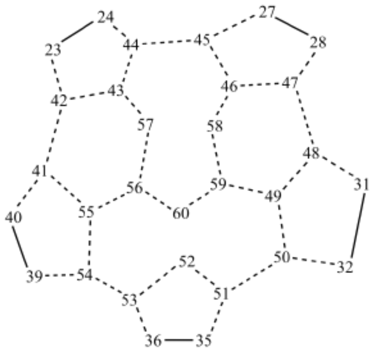
6,7-seco-1,2,3,9,12,15-hexanor(C_{60}-I_h)[5,6]fullerene (PIN)

Explanation: The preferred IUPAC name for this fullerene fragment is a seconorfullerene name because it has 54 carbon atoms and 22 rings.

Example 2: $C_{30}H_{14}$


17
20
16
18
19
21
12
13
2
3
14
1
11a
3a
14a
15a
11
$9a^1$
15
$3a^1$
4
22
10
9a
5a
5
9
6
8
7

(**I**)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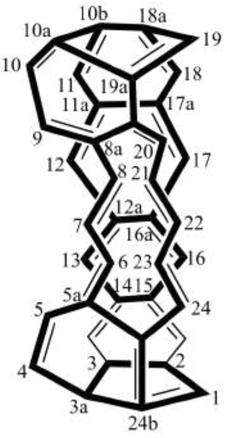
(**II**)

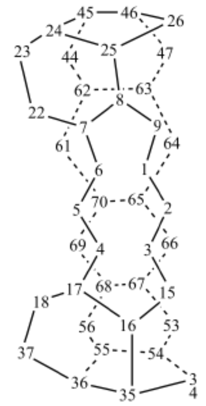
3,2,13,12-(epihexa[1,3,5]trien[1,3,4,6]tetrayl)-6,9-methenocycloundeca[1,11,10-*cd*:6,7,8-*c′d′*]diindene (**I**) (PIN)
[not 57,58:52,60-diseco-1,2,3,4,5,6,7,8,9,10,11,12,13,14,15,16,17,18,19,20,21,22,25,26,29,30,33,34,37,38-triacontanor(C_{60}-I_h)[5,6]fullerene (**II**)]

Explanation: The preferred IUPAC name for this fullerene fragment is a systematic bridged fused ring name because it has 30 carbon atoms and only 7 five- and six-membered rings.

Example 3: $C_{40}H_{20}$


10b
18a
10a
19
10
18
11
19a
11a
17a
9
8a
20
12
8
21
17
12a
7
16a
22
13
6
23
16
14
15
5a
24
5
3
2
4
3a
1
24b

(**I**)


45
46
26
24
23
44
25
47
62
63
8
22
7
9
61
64
6
1
70
65
5
2
69
4
3
66
17
68
67
15
18
56
16
53
55
54
37
36
35
34

(**II**)

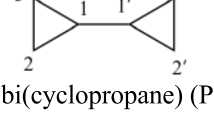
2,15:3,14-dimethenoindeno[5″,4″:6′,7′]cyclododeca[1′,2′:4,5]indeno[1,2-*b*]anthracene (**I**) (PIN)
[not 1,6:3,4-diseco-10,11,12,13,14,19,20,21,27,28,29,30,31,32,33,38,39,40,41,42,43,48,49,50,51,52,57,58,59,60-triacontanor(C_{70}-$D_{5h(6)}$)[5,6]fullerene (**II**)]

Explanation: The preferred IUPAC name for this fullerene fragment is a systematic fused ring name because it contains 40 carbon atoms but only eight five- and six-membered rings.

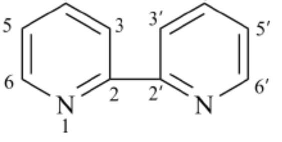
P-52.2.7 Preferred IUPAC names and numbering for ring assemblies

P-52.2.7.1 Preferred IUPAC names for assemblies of two or more identical cyclic systems joined by a single bond are formed using the names of parent hydrides rather than the names of substituent groups, except for biphenyl and polyphenyl assemblies, for which the name benzene is never used. For two-component assemblies, locants of one ring are unprimed; locants of the second ring are primed. Locants, including the locants 1 and 1′, are necessary in preferred IUPAC names to indicate points of attachment of rings or ring systems (see P-28.2.1).

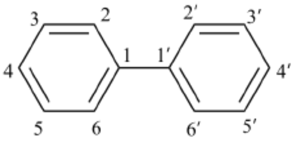
Examples:



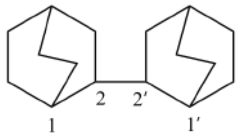
1,1′-bi(cyclopropane) (PIN)
1,1′-bi(cyclopropyl)


4
4′
5
3
3′
5′
6
N
1
2
2′
N
6′

2,2′-bipyridine (PIN)
2,2′-bipyridyl



1,1′-biphenyl (PIN)
biphenyl

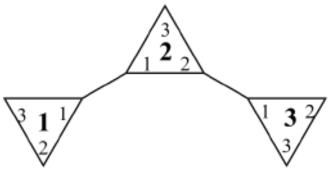


2,2′-bi(bicyclo[2.2.2]octane) (PIN)
2,2′-bi(bicyclo[2.2.2]octanyl)

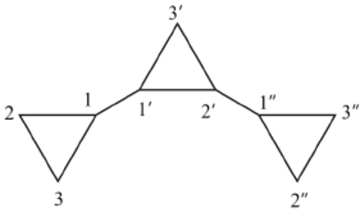
P-52.2.7.2 The preferred numbering for ring assemblies composed of three or more identical cyclic systems uses composite locants rather than primed locants (see P-28.3.1).

A new numbering system is now recommended for preferred IUPAC names of ring assemblies with more than two rings or ring systems; it consists of composite locants, for example, 1^2. The previously used locant system for ring assemblies with more than two rings or ring systems using serially primed locants (refs. 1 and 2) may be used in general nomenclature.

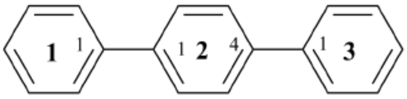
Examples:



$1^1,2^1:2^2,3^1$-tercyclopropane (PIN)



1,1′:2′,1″-tercyclopropane

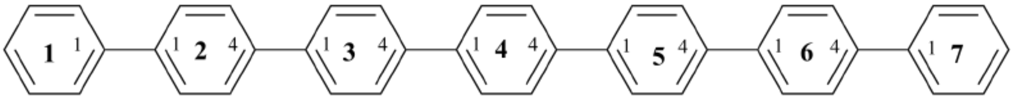


$1^1,2^1:2^4,3^1$-terphenyl (PIN)
1,1′:4′,1″-terphenyl
(not *p*-terphenyl)

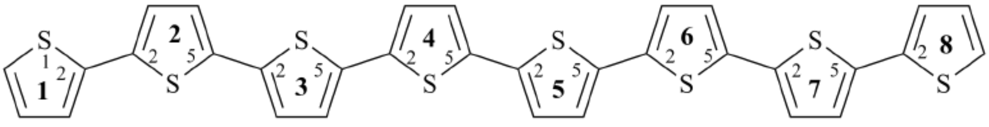
P-52.2.7.3 Preferred IUPAC names for assemblies containing seven and more rings or ring systems.

Phane names are preferred IUPAC names rather than ring assembly names when seven or more rings or ring systems are present.

Examples:



1,7(1),2,3,4,5,6(1,4)-heptabenzenaheptaphane (PIN)
$1^1,2^1:2^4,3^1:3^4,4^1:4^4,5^1:5^4,6^1:6^4,7^1$-septiphenyl
1,1′:4′,1″:4″,1‴:4‴,1‴ ′:4‴ ′,1‴ ″:4‴ ″,1‴ ‴-septiphenyl

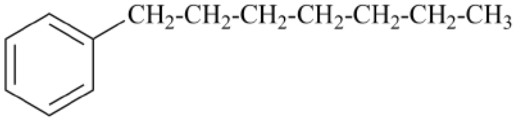


1,8(2),2,3,4,5,6,7(2,5)-octathiophenaoctaphane (PIN)
$1^2,2^2:2^5,3^2:3^5,4^2:4^5,5^2:5^5,6^2:6^5,7^2,7^5,8^2$-octithiophene
2,2′:5′,2″:5″,2‴:5‴,2‴ ′:5‴ ′,2‴ ″:5‴ ″,2‴ ‴:5‴ ‴,2‴ ‴ ′-octithiophene

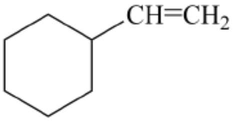
P-52.2.8 Selection between a ring and a chain as parent hydride

Within the same heteroatom class and for the same number of characteristic groups cited as the principal characteristic group, a ring is always selected as the parent hydride to construct a preferred IUPAC name. In general nomenclature, a ring or a chain can be the parent hydride (see P-44.1.2.2).

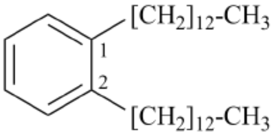
Examples:



(a) heptylbenzene (PIN) (ring preferred to chain)
(b) 1-phenylheptane (chain has greater number of skeletal atoms)



(a) ethenylcyclohexane (PIN) (ring preferred to chain)
(b) cyclohexylethene (emphasizes unsaturation)



1,2-di(tridecyl)benzene (PIN) (ring preferred to chain)
[not 1,1′-(1,2-phenylene)di(tridecane);
multiplication of acyclic hydrocarbons is not allowed]

P-53 SELECTING PREFERRED RETAINED NAMES OF PARENT HYDRIDES

A certain number of retained names of parent hydrides are still recommended. The names methane, ethane, propane, and butane have been used since the beginning of systematic nomenclature. Names of cyclic mancude compounds are retained as components of fusion nomenclature; they are also used as preferred IUPAC names to name their derivatives and in general nomenclature.

An important aspect of these retained names is their substitutability; as parent compounds, they accommodate without restriction substituent groups cited as suffixes and prefixes. A few are limited in their capacity to be substituted; amongst them are the substituted benzenes ‘toluene’, ‘xylene’, and ‘mesitylene’. Some retained names are no longer recommended, for example ‘cumene’ and ‘cymene’.

For preferred retained IUPAC names of parent hydrides, see P-21.1.1 and P-21.1.2 for acyclic parent hydrides, P-22.1 and P-22.2 for monocyclic parent hydrides and P-25.1 and P-25.2 for polycyclic parent hydrides.

P-54 SELECTING THE PREFERRED METHOD FOR MODIFYING THE DEGREE OF HYDROGENATION

P-54.1 METHODS FOR MODIFYING

THE DEGREE OF HYDROGENATION OF PARENT HYDRIDES

There are three methods for modifying the degree of hydrogenation for parent hydrides:

(1) by changing the ending ‘ane’ in acyclic parent hydrides to ‘ene’ and ‘yne’;

(2) by using ‘hydro’ prefixes to saturate one or more double bonds in mancude compounds;

(3) by using ‘dehydro’ prefixes to introduce triple bonds in mancude compounds (see P-54.4).

Systematic IUPAC names and retained names of parent hydrides may be modified in the same way or in different ways to generate preferred IUPAC names.

P-54.2 UNSATURATED MONOCYCLIC CARBOCYCLES

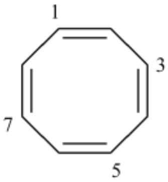
Two methods are used for modifying the degree of hydrogenation of monocyclic carbocycles:

(1) by using the endings ‘ene’ and ‘yne’;

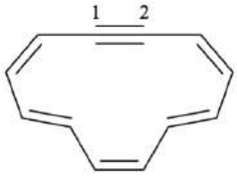
(2) by using the parent name ‘annulene’.

Method (1) generates preferred IUPAC names:

Examples:



cycloocta-1,3,5,7-tetraene (PIN)
[8]annulene

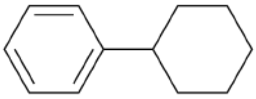


(1*Z*,3*E*,5*Z*,7*E*,9*Z*)-cyclododeca-1,3,5,7,9-pentaen-11-yne (PIN)
1,2-didehydro[12]annulene (numbering shown)

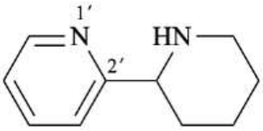
P-54.3 UNSATURATION IN RING ASSEMBLIES COMPOSED OF MONOCYCLIC MANCUDE AND SATURATED RINGS

When assemblies of otherwise identical rings contain both mancude and saturated rings, the use of hydro prefixes is preferred, except in the case of a two ring assembly consisting of one benzene ring and a cyclohexane ring. However, when the requirements for the formation of phane names are met (see P-52.2.5.1), phane names are preferred IUPAC names.

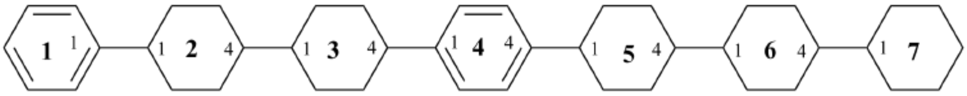
Examples:



cyclohexylbenzene (PIN)
1,2,3,4,5,6-hexahydro-1,1′-biphenyl



1,2,3,4,5,6-hexahydro-2,2′-bipyridine (PIN)
2-(piperidin-2-yl)pyridine



1(1),4(1,4)-dibenzena-2,3,5,6(1,4),7(1)-pentacyclohexanaheptaphane (PIN)
1^4-[4-(4′-phenyl[1,1′-bi(cyclohexan)]-4-yl)phenyl]-1^1,2^1:2^4,3^1-tercyclohexane

P-54.4 NAMES MODIFIED BY ‘HYDRO’ AND ‘DEHYDRO’ PREFIXES

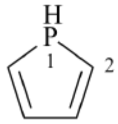
In these recommendations, the prefixes ‘hydro’ and ‘dehydro’ are detachable, but are not included in the category of alphabetized detachable prefixes (see P-14.4; see also P-15.1.5.2, P-31.2, P-58.2), which is a change from recommendations in earlier editions (ref. 1, 2) where they were alphabetized along with substituent prefixes. When along with the endings ‘ene’ and ‘yne’ they are used to modify parent hydrides, they are regulated by the principle of lowest locants, in accord with the numbering of the parent hydride and after priority has been given to indicated hydrogen, added indicated hydrogen, and suffixes, when present, as specified in the general rules for numbering (P-14.4).

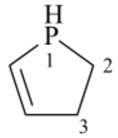
P-54.4.1 Hantzsch-Widman heteromonocycles

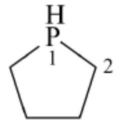
Preferred IUPAC names for Hantzsch-Widman rings correspond to either fully unsaturated or fully saturated compounds (see P-22.2.2.1.1). ‘Hydro’ prefixes added to names of fully unsaturated Hantzsch-Widman rings lead to preferred IUPAC names for partially unsaturated rings; names containing the ‘dehydro’ prefix are allowed only in general nomenclature.

The final ‘e’ in Hantzsch-Widman names is required in preferred IUPAC names; it is still optional in general nomenclature. In the 1979 Rules (ref. 1), the final ‘e’ of a Hantzsch-Widman name was omitted when there was no nitrogen in the ring; in the 1993 Guide (ref. 2) this omission was made optional.

Examples:


1*H*-phosphole (PIN)

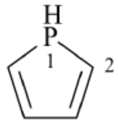

2,3-dihydro-1*H*-phosphole (PIN)
2,3-didehydrophospholane

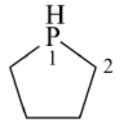

phospholane (PIN)

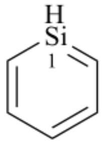
P-54.4.2 Saturated heteromonocyclic compounds

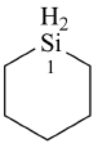
Preferred IUPAC names for saturated heteromonocyclic compounds are either Hantzsch-Widman names described in P-22.2.2.1.1 or retained names given in Table 2.3. Names of saturated rings derived by using hydro prefixes with Hantzsch-Widman names (see P-54.4.1) and retained names by adding the maximum of hydro prefixes, or 'cyclo' names described in P-22.2.5, are not preferred IUPAC names, but they may be used in general nomenclature.

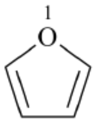
Examples:

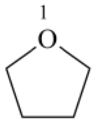

1*H*-phosphole (PIN)

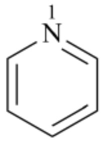

phospholane (PIN)
2,3,4,5-tetrahydro-1*H*-phosphole

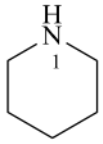

siline (PIN)

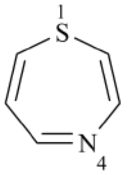

silinane (PIN)
hexahydrosiline

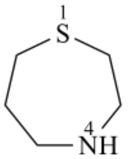

furan (PIN)

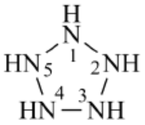

oxolane (PIN)
tetrahydrofuran


pyridine (PIN)


piperidine (PIN)
hexahydropyridine


1,4-thiazepine (PIN)


1,4-thiazepane (PIN)
hexahydro-1,4-thiazepine

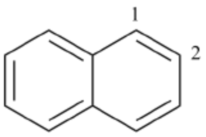

cylopentaazane
pentazolidine (preselected name; see P-22.2.2.1.2)

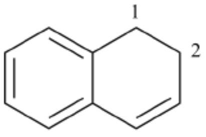
P-54.4.3 Fused ring systems and mancude ring assemblies composed of fused ring systems

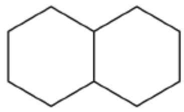
P-54.4.3.1 Retained fusion names are used for the fully unsaturated compounds (see P-25); they are the preferred IUPAC names. Preferred IUPAC names for the partially saturated and fully saturated compounds are formed by using 'hydro' prefixes. Preferred IUPAC names for partially saturated and mancude ring assemblies are formed in the same way.

In these recommendations, the prefix 'hydro' is detachable, but is not included in the category of alphabetized detachable prefixes (see P-14.4; see also P-15.1.5.2, P-31.2, P-58.2), which is a change from recommendations in earlier editions (ref. 1, 2) where it was alphabetized along with prefixes. When along with the endings 'ene' and 'yne' it is used to modify parent hydrides, it is regulated by the principle of lowest locants, in accord with the numbering of the parent hydride and after priority has been given to indicated hydrogen, added indicated hydrogen, and suffixes, when present, as specified in the general rules for numbering (P-14.4).

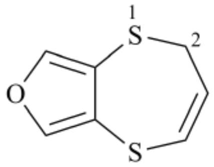
Examples:


naphthalene (PIN)

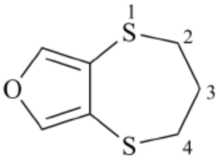

1,2-dihydronaphthalene (PIN)



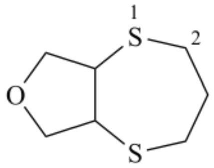
decahydronaphthalene (PIN)
bicyclo[4.4.0]decane



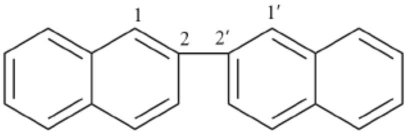
2*H*-[1,4]dithiepino[2,3-*c*]furan (PIN)



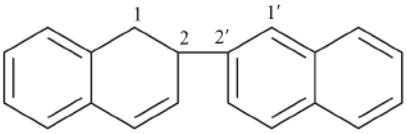
3,4-dihydro-2*H*-[1,4]dithiepino[2,3-*c*]furan (PIN)



hexahydro-2*H*-[1,4]dithiepino[2,3-*c*]furan (PIN)



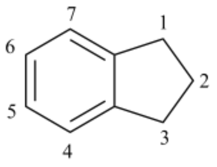
2,2′-binaphthalene (PIN)
2,2′-binaphthyl



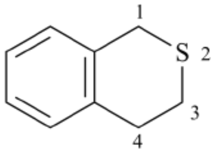
1,2-dihydro-2,2′-binaphthalene (PIN)
1,2-dihydro-2,2′-binaphthyl
1,2-dihydro-2-(naphthalen-2-yl)naphthalene

P-54.4.3.2 The retained names for the partially saturated heterocycles, ‘indane’, ‘indoline’, ‘isoindoline’, and ‘chromane’, ‘isochromane’ and their chalcogen analogues are not used as preferred IUPAC names, but are acceptable for use in general nomenclature (see P-31.2.3.3.1). Preferred IUPAC names are based on the retained mancude names indene, 1*H*-indole, 1*H*-isoindole, 2*H*-1-benzopyran, and 1*H*-2-benzopyran (and their chalcogen analogues) modified by ‘hydro’ prefixes (see P-54.4.3.1).

Example:



indane
2,3-dihydro-1*H*-indene (PIN)



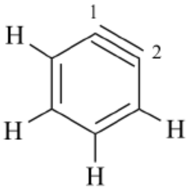
isothiochroman
3,4-dihydro-1*H*-2-benzothiopyran (PIN)

P-54.4.4 Names modified by ‘dehydro’ prefixes

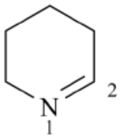
‘Dehydro’ prefixes are used to generate preferred IUPAC names for dehydrogenated mancude compounds. They may be used in general nomenclature to introduce double and triple bonds in saturated parent hydrides.

In these recommendations, the prefix ‘dehydro’ is detachable, but is not included in the category of alphabetized detachable prefixes (see P-14.4; see also P-15.1.5.2, P-31.2, P-58.2), which is a change from recommendations in earlier editions (ref. 1, 2) where it was alphabetized along with substituent prefixes. When along with the endings ‘ene’ and ‘yne’ it is used to modify parent hydrides it is regulated by the principle of lowest locants, in accord with the numbering of the parent hydride and after priority has been given to indicated hydrogen, added indicated hydrogen, and suffixes, when present, as specified in the general rules for numbering (P-14.4).

Examples:



1,2-didehydrobenzene (PIN)
cyclohexa-1,3-dien-5-yne
(not benzyne)



1,2-didehydropiperidine
2,3,4,5-tetrahydropyridine (PIN)

P-55 SELECTING THE PREFERRED RETAINED NAME FOR FUNCTIONAL PARENT COMPOUNDS

Trivial names retained for naming organic compounds are known as ‘retained names’. Parent hydrides and functional parent compounds may have retained names. The number of parent hydrides having retained names has been kept almost unchanged through the years. The main reason is that the aliphatic ones methane, ethane, propane and butane have been in use since the Geneva Convention; most of the cyclic parent hydrides are used as components in systematic fusion nomenclature as discussed in Section P-52. The situation regarding functional parent compounds is different. Their number was sharply reduced in the 1979 Rules, and reduced still further in the 1993 Recommendations. In these recommendations, their usage as preferred IUPAC names has been sharply limited. All retained names in the 1993 list can be used in general and specialized nomenclature. Two distinct classes are thus recognized.

(1) Retained names used as preferred IUPAC names.

(2) Retained names recommended for general nomenclature.

A further classification regarding substitution was established in the 1993 Recommendations. Structures corresponding to retained names could be substituted without restriction, substituted in a limited way, or simply could not be substituted at all. This issue is discussed in P-15.1.8.

In the context of preferred IUPAC names, most parent hydrides having retained names recommended as preferred IUPAC names are fully substitutable and most functional parent compounds having retained names also recommended as preferred IUPAC names can be substituted, albeit in the limited way imposed by the presence of a characteristic group and the seniority of classes. Exceptions are known, when no substitution is allowed.
Retained names recommended for general and specialized nomenclature must be used as in the past. Rules about substitution of corresponding structures are less strict and traditional IUPAC nomenclature can still be applied in all its diversity and adaptability. In this Section, preferred IUPAC names only will be discussed.

Organic functional parent compounds having retained names used as preferred IUPAC names are all listed in P-34.1. Substitution is allowed on all structures except anisole and *tert*-butoxy, and formic acid and formyl group are substitutable with limitations.

For inorganic parent compounds, see P-67.1.2 and P-67.2.1. Organic functional parent compounds for general nomenclature, see P-34.1.3.

P-56 SELECTING THE PREFERRED SUFFIX FOR THE PRINCIPAL CHARACTERISTIC GROUP

Suffixes have always been considered as the most unique elements of the formation of names. In the past, some suffixes have been discarded and replaced by new ones. The following suffixes have been introduced or modified in these recommendations.

P-56.1 THE SUFFIX 'PEROXOL', FOR –OOH

It is now recommended to use the sufix 'peroxol' to provide substitutive names for hydroperoxides. Such names are preferred to those generated by functional class nomenclature.

> The suffix 'peroxol' for –OOH is now adopted to name hydroperoxides, which in previous recommendations were named by functional class nomenclature.

Example:

CH_3-CH_2-OOH
ethaneperoxol (PIN)
ethyl hydroperoxide

P-56.2 THE SUFFIXES '*SO*-THIOPEROXOL', AND CHALOGEN ANALOGUES

The suffix 'sulfenic acid' and its chalcogen analogues were discarded in the 1993 recommendations (ref. 2). In these recommendations, these suffixes are replaced by the new suffixes, '*SO*-thioperoxol', '*SeO*-selenoperoxol', 'dithioperoxol', '*TeS*-tellurothioperoxol', 'diselenoperoxol', '*SeTe*-selenotelluroperoxol' and '*TeSe*-telluroselenoperoxol' (see P-63.4.2.1).

> The suffixes *SO*-thioperoxol and its chalcogen analogues are now introduced to replace the suffix 'sulfenic acid' and its chalcogen analogues that were discarded in the 1993 recommendations.

Examples:

CH_3-S-OH
methane-*SO*-thioperoxol (PIN)
(not methanesulfenic acid)

C_6H_5-SeSe-H
benzenediselenoperoxol (PIN)
(not benzeneselenoselenic acid)

P-56.3 THE SUFFIXES 'IMIDAMIDE' AND 'CARBOXIMIDAMIDE'

The suffixes 'amidine' and 'carboxamidine', for –C(=NH)-NH_2 and –(C)(=NH)-NH_2, are no longer recommended. They are replaced by the new functional replacement suffixes 'imidamide' and 'carboximidamide' in preferred IUPAC names (see P-66.4.1).

Examples:

CH_3-C(=NH)-NH_2
ethanimidamide (PIN)
(no longer acetamidine)
C_6H_{11}-C(=NH)-NH_2
cyclohexanecarboximidamide (PIN)
(no longer cyclohexanecarboxamidine)

P-56.4 THE ENDINGS 'DIYL' AND 'YLIDENE' *VS.* 'YLENE'

Except for 'methylene', 'ethylene', and 'phenylene', the suffix 'ylene' previously used to describe divalent substituent groups in which the free valences do not form a double bond, i.e., –E– or E< was discarded in 1993 (ref. 2). Substituent groups in which the free valences form a double bond, i.e., E= were described by the suffix 'ylidene'. The suffix 'ylene' was replaced by the suffixes 'diyl' to express the –E– or E< type of bonding, and 'ylidene' for E=, for example, ethane-1,2-diyl for –CH_2-CH_2– and ethylidene for H_3C-CH=, respectively. However, the name 'methylene' is retained to describe the substituent group –CH_2–; it is used in preferred IUPAC names rather than methanediyl. CAS still use the 'ylene' suffix to describe the 'diyl' and 'ylidene' types of bonds, especially 'methylene' for –CH_2– and CH_2=.

Examples:

–CH_2–	H_2C=
methylene (preferred prefix)	methylidene (preferred prefix)
(not methanediyl)	(formerly methylene)

$–CH_2\text{-}CH_2–$
ethane-1,2-diyl (preferred prefix)
ethylene

$CH_3\text{-}CH=$
ethylidene (preferred prefix)

$–SiH_2–$
silanediyl (preselected prefix)
(not silylene,
a name still used by CAS)

$H_2Ge=$
germylidene (preselected prefix)
(not germylene,
a name still used by CAS)

$–BH–$
boranediyl (preselected prefix)
(not borylene,
a name still used by CAS)

$HB=$
boranylidene (preselected prefix)
(not borylene,
a name still used by CAS)

$–SbH–$
stibanediyl (preselected prefix)
(not stibinediyl)
(not stibylene,
a name still used by CAS)

$HSb=$
stibanylidene (preselected prefix)
(not stibinylidene)
(not stibylene,
a name still used by CAS)

–NH-CO-NH–
carbonylbis(azanediyl) [preferred prefix,
a name used in multiplicative nomenclature; (see P-66.1.6.1.1.3)]
(not carbonyldiimino,
a name still used by CAS)
(not ureylene)

P-57 SELECTING PREFERRED AND PRESELECTED PREFIXES FOR SUBSTITUENT GROUPS

Preferred prefixes for substituent groups are considered here in three different sections. A comprehensive list is provided in Appendix 2.

All substituent groups are named systematically using substitutive nomenclature. Some names are retained; they are important because they do have priority over systematic substitutive names.

P-57.1 Prefixes derived from parent hydrides
P-57.2 Prefixes derived from characteristic (functional) groups
P-57.3 Prefixes derived from functional parent compounds
P-57.4 Construction of linear compound and/or complex substituent prefixes.

P-57.1 PREFIXES DERIVED FROM PARENT HYDRIDES

P-57.1.1 Prefixes derived from mononuclear and acyclic parent hydrides

P-57.1.1.1 When the free valences are in position 1 of substituent groups derived from mononuclear hydrides carbon, silicon, germanium, tin and lead and from acyclic hydrocarbons, preferred prefixes are of the ‘alkyl type’ according to P-29.2; preferred prefixes are of the ‘alkanyl type’ for all mononuclear hydrides other than those mentioned above and for saturated substituent groups when the free valences are not in position 1.

Examples:

$CH_3–$
methyl (preferred prefix)
methanyl

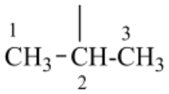
$PH_2–$
phosphanyl (preselected prefix)

$SiH_3–$
silyl (preselected prefix)
silanyl

$CH_3\text{-}CH_2\text{-}\overset{1}{C}H=$
propylidene (preferred prefix)
propan-1-ylidene

$CH_2=$
methylidene (preferred prefix)
methanylidene

$CH_3\text{-}C\equiv$
ethylidyne (preferred prefix)
ethanylidyne



$$\overset{1}{C}H_3\text{-}\underset{2}{\overset{|}{C}}H\text{-}\overset{3}{C}H_3$$

propan-2-yl (preferred prefix)
1-methylethyl
isopropyl

$$H_3\overset{3}{Si}\text{-}\overset{2}{Si}H_2\text{-}\overset{1}{Si}H_2\text{–}$$

trisilan-1-yl (preselected prefix)

P-57.1.1.2 The prefix methylene is retained as a preferred prefix with unlimited substitution except for substituents that would create a carbon chain.

P-57.1.2 The following retained names are used as preferred prefixes for which no substitution is recommended:

Examples:

$\text{–}C(CH_3)_3$
tert-butyl (preferred prefix)
1,1-dimethylethyl

$C_6H_5\text{-}CH_2\text{–}$
benzyl (preferred prefix)
phenylmethyl

$C_6H_5\text{-}CH=$
benzylidene (preferred prefix)
phenylmethylidene

$C_6H_5\text{-}C\equiv$
benzylidyne (preferred prefix) phenylmethylidyne

> For preferred prefixes, the names 'benzyl', 'benzylidene', and 'benzylidyne' cannot be substituted. Previously, in the 1993 Guide (ref. 2), they could only be substituted on the ring. However, for general nomenclature restricted substitution is permitted (see P-29.6.2.1).

P-57.1.3 Retained prefixes recommended only for general nomenclature

The prefix 'ethylene', for $\text{–}H_2C\text{-}CH_2\text{–}$, is recommended, with unlimited substitution, only for general nomenclature (P-29.6.2.3).

Isopropyl for $(CH_3)_2CH\text{–}$, isopropylidene for $(CH_3)_2C=$, and trityl for $(C_6H_5)_3C\text{–}$ are retained as prefixes only for use in general nomenclature but no substitution of any kind is allowed (see P-29.6.2.2).

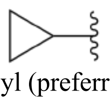
P-57.1.4 Retained prefixes no longer recommended

The retained names phenethyl (2-phenylethyl) for $C_6H_5\text{-}CH_2\text{-}CH_2\text{–}$; benzhydryl (diphenylmethyl), for $(C_6H_5)_2CH\text{–}$; isobutyl (2-methylpropyl) for $(CH_3)_2CH\text{-}CH_2\text{–}$; *sec*-butyl (butan-2-yl, 1-methylpropyl) for $CH_3\text{-}CH_2\text{-}CH(CH_3)\text{–}$; isopentyl (3-methylbutyl) for $(CH_3)_2CH\text{-}CH_2\text{-}CH_2\text{–}$; *tert*-pentyl (2-methylbutan-2-yl, 1,1-dimethylpropyl) for $CH_3\text{-}CH_2\text{-}C(CH_3)_2\text{–}$; and neopentyl (2,2-dimethylpropyl) for $(CH_3)_3C\text{-}CH_2\text{–}$; are no longer recommended; the first name in parentheses is the preferred prefix name.

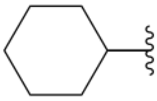
P-57.1.5 Prefixes derived from cyclic parent hydrides

P-57.1.5.1 Preferred prefixes derived from cycloalkanes are of the 'cycloalkyl type' (see P-29.2); preferred prefixes derived from cyclic compounds other that cycloalkanes are all of the 'alkanyl type' described above in P-57.1.1.1.

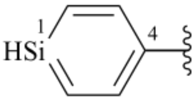
Examples:



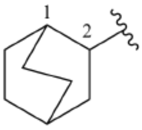
cyclopropyl (preferred prefix)
cyclopropanyl



cyclohexyl (preferred prefix)
cyclohexanyl



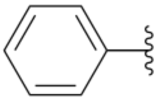
silin-4-yl (preferred prefix)



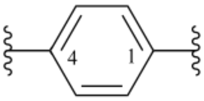
bicyclo[2.2.2]octan-2-yl (preferred prefix)
bicyclo[2.2.2]oct-2-yl

P-57.1.5.2 Retained prefixes used as preferred prefixes (see P-29.6.1)

The two following prefixes are retained as preferred prefixes with unlimited substitution:



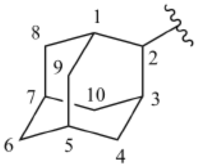
phenyl (preferred prefix)



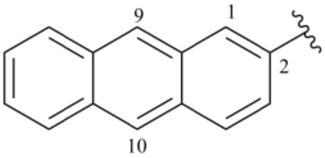
1,4-phenylene (also 1,2- and 1,3-isomers)
(preferred prefixes)

P-57.1.5.3 Retained prefixes recommended only for use in general nomenclature (P-29.6.2.3).

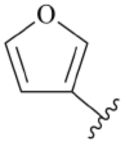
The following retained prefixes are recommended for only general nomenclature, with unlimited substitution except for tolyl for which no substitution is allowed:



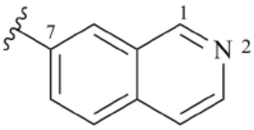
2-adamantyl (also 1-isomer)
adamantan-2-yl (preferred prefix)



2-anthryl (also 1- and 9-isomers)
anthracen-2-yl (preferred prefixes)

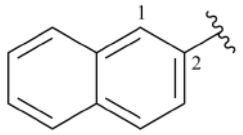


3-furyl (also 2-isomer)
furan-3-yl (also 2-isomer;
preferred prefixes)

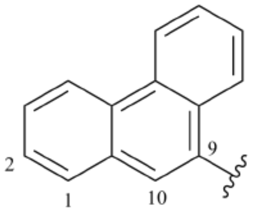


7-isoquinolyl (also 1-, 3-, 4-, 5-, 6- and 8-isomers)

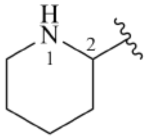
isoquinolin-7-yl (also 1-, 3-, 4-, 5-, 6- and 8-isomers,
preferred prefixes)



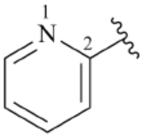
2-naphthyl (also 1-isomer)
naphthalen-2-yl (also 1-isomer;
preferred prefixes)



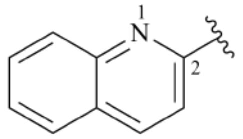
9-phenanthryl (also 1-, 2-, 3- and 4-isomers)
phenanthren-9-yl (also 1-, 2-, 3- and 4-isomers,
preferred prefixes)



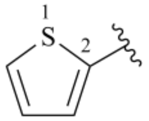
2-piperidyl (also 3- and 4-isomers)
piperidin-2-yl (also 3- and 4-isomers;
preferred prefixes)



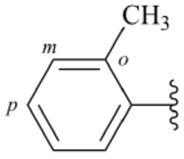
2-pyridyl (also 3- and 4-isomers)
pyridin-2-yl (also 3- and 4-isomers;
preferred prefixes)



2-quinolyl (also 3-, 4-, 5-, 6-, 7- and 8-isomers)
quinolin-2-yl (also 3-, 4-, 5-, 6-, 7- and 8-isomers;
preferred prefixes)



2-thienyl (also 3-isomer)
thiophen-2-yl (also 3-isomer;
preferred prefixes)



o-tolyl (also *m*- and *p*-isomers;
no substitution allowed)
2-methylphenyl (also 3- and 4-isomers;
preferred prefixes)

P-57.1.5.4 Retained prefixes that are no longer recommended

The retained prefixes furfuryl (2 isomer only) and thenyl (2 isomer only) are no longer recommended (see P-29.6.3)

P-57.1.6 Prefixes derived from parent hydrides with modified degrees of hydrogenation

P-57.1.6.1 All preferred prefixes derived from parent hydrides whose degree of hydrogenation has been modified are formed systematically according to rules discussed in P-32. There is a choice when the free valences are in position 1 or at any position on the chain: preferred prefixes are given to the less substituted chain (see example 3 below, and many examples in P-32.1.1).

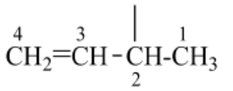
Examples:

$\overset{4}{\mathrm{CH_2}}=\overset{3}{\mathrm{CH}}-\overset{2}{\mathrm{CH_2}}-\overset{1}{\mathrm{CH_2}}-$

but-3-en-1-yl (preferred prefix)

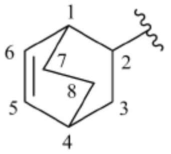
$\overset{3}{\mathrm{CH_2}}=\overset{2}{\mathrm{CH}}-\overset{1}{\mathrm{CH_2}}-$

prop-2-en-1-yl (preferred prefix)

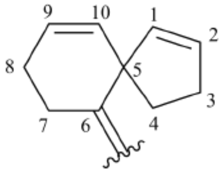


$\overset{4}{\mathrm{CH_2}}=\overset{3}{\mathrm{CH}}-\underset{2}{\overset{|}{\mathrm{CH}}}-\overset{1}{\mathrm{CH_3}}$

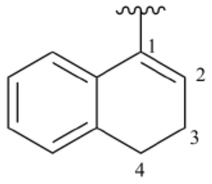
but-3-en-2-yl (preferred prefix)
1-methylprop-2-en-1-yl



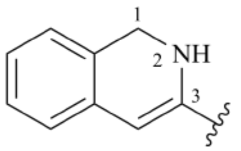
bicyclo[2.2.2]oct-5-en-2-yl (preferred prefix)



spiro[4.5]deca-1,9-dien-6-ylidene (preferred prefix)



3,4-dihydronaphthalen-1-yl (preferred prefix)



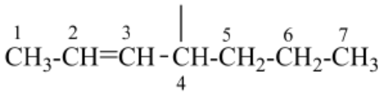
1,2-dihydroisoquinolin-3-yl (preferred prefix)

P-57.1.6.2 Two important changes from previous recommendations involving prefixes derived from parent hydrides with modified degrees of hydrogenation must be noted.

(1) In acyclic prefixes, the longest chain is chosen as the principal chain;

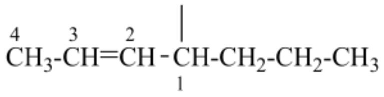
In these recommendations, a major change in the naming of substituents derived from unsaturated acyclic compounds is adopted in which the longest chain is chosen as the parent chain regardless of the number or type of multiple bonds.

Examples:



$\overset{1}{\mathrm{CH_3}}-\overset{2}{\mathrm{CH}}=\overset{3}{\mathrm{CH}}-\underset{4}{\overset{|}{\mathrm{CH}}}-\overset{5}{\mathrm{CH_2}}-\overset{6}{\mathrm{CH_2}}-\overset{7}{\mathrm{CH_3}}$

hept-2-en-4-yl [alkanyl type;
see P-29.2 method (2)]
(preferred prefix)



$\overset{4}{\mathrm{CH_3}}-\overset{3}{\mathrm{CH}}=\overset{2}{\mathrm{CH}}-\underset{1}{\overset{|}{\mathrm{CH}}}-\mathrm{CH_2}-\mathrm{CH_2}-\mathrm{CH_3}$

1-propylbut-2-en-1-yl [alkyl type;
see P-29.2 method (1)]

(2) In acyclic prefixes derived from alkanes modified by skeletal replacement (‘a’) nomenclature, the ‘a’ prefixes have seniority over suffixes, such as ‘yl’ and ‘ylidene’.

Fixed numbering for heteroacyclic parent structures named by skeletal replacement (‘a’) nomenclature is a major change to Rule C-0.6 (ref. 1) where principal characteristic groups and free valence were preferred over heteroatoms for low locants.

Example:

$$\overset{1}{CH_3}\text{-}\overset{2}{O}\text{-}\overset{3}{CH_2}\text{-}\overset{4}{CH_2}\text{-}\overset{5}{O}\text{-}\overset{6}{CH_2}\text{-}\overset{7}{CH_2}\text{-}\overset{8}{O}\text{-}\overset{9}{CH_2}\text{-}\overset{10}{CH_2}\text{-}\overset{11}{O}\text{-}\overset{12}{CH}\text{=}\overset{13}{CH}\text{–}$$

2,5,8,11-tetraoxatridec-12-en-13-yl (preferred prefix)
(not 3,6,9,12-tetraoxatridec-1-en-1-yl;
the suffix ‘-yl’ is added to the parent hydride name 2,5,8,11-tetraoxatridecane)

P-57.1.6.3 Retained prefixes derived from parent hydrides with modified degrees of hydrogenation

There are no retained prefixes derived from parent hydrides with a modified degree of hydrogenation recommended as preferred prefixes. The retained prefixes vinyl (ethenyl), for CH_2=CH–; vinylidene (ethenylidene), for CH_2=C=; allyl (prop-2-en-1-yl), for $\overset{3}{CH_2}\text{=}\overset{2}{CH}\text{-}\overset{1}{CH_2}\text{–}$; allylidene (prop-2-en-1-ylidene), for $\overset{3}{CH_2}\text{=}\overset{2}{CH}\text{-}\overset{1}{CH}\text{=}$; and allylidyne (prop-2-en-1-ylidyne) for CH_2=CH-C≡; are retained but only for general nomenclature (see P-32.3). Substitution is allowed, but not by alkyl or any other group that extends the carbon chain or by characteristic groups expressed by suffixes. The preferred prefixes are given in parentheses.

The prefix isopropenyl (prop-1-en-2-yl), for CH_2=C(CH_3)–, is a retained prefix but is not used as a preferred prefix. It is acceptable for general use but no substitution is allowed. The preferred prefix is given in parentheses.

The prefixes indan-2-yl, indolin-2-yl, isoindolin-2-yl, chroman-2-yl and isochroman-2-yl, as well as other isomers, are recommended for general nomenclature only, with unlimited substitution (see Table 3.2).

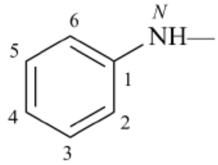
P-57.2 PREFIXES DERIVED FROM CHARACTERISTIC (FUNCTIONAL) GROUPS

Names of prefixes derived from characteristic groups are either retained names or are systematically formed by substitutive nomenclature. Retained prefixes are described in P-35.2.1 and P-35.2.3. Substitutive systematic prefixes are formed by the general methodology described for prefixes derived from parent hydrides (see P-57.1.1). In fact, prefixes derived from characteristic groups are those derived from parent hydrides of Groups 17, 16 and from azane in Group 15; they are discussed in P-35.2.2.

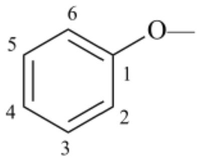
P-57.3 PREFIXES DERIVED FROM ORGANIC FUNCTIONAL PARENT COMPOUNDS

Names of prefixes derived from functional parent compounds are either retained prefixes or are systematically formed by substitutive nomenclature. Retained prefixes corresponding to functional parent compounds used as preferred prefixes are described in P-34.2. Retained prefixes derived from functional compounds that can only be used in general nomenclature are described in Chapter P-6 in Sections related to specific classes. Appendix 2 contains all prefixes derived from functional parent hydrides.

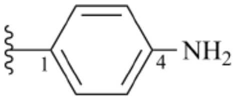
Examples:



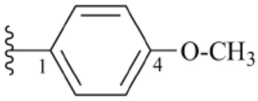
anilino (preferred prefix)
(a retained simple prefix derived from aniline;
full substitution is allowed; see P-34.2.1.3)
phenylamino



phenoxy (preferred prefix)
(a retained simple prefix derived from phenol;
substitution allowed; see P-63.2.2.2)



4-aminophenyl (preferred prefix)
(a systematic compound prefix)



4-methoxyphenyl (preferred prefix)
(a systematic compound prefix)

H-CO–
formyl (preferred prefix,
see P-65.1.7.2.1)

CH_3-CO–
acetyl (preferred prefix,
see P-65.1.7.2.1)

P-57.4 CONSTRUCTION OF LINEAR COMPOUND AND/OR COMPLEX SUBSTITUENT PREFIXES.

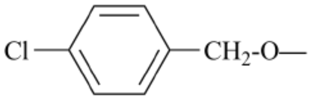
Linear compound and complex prefixes are constructed in a stepwise manner by working backwards component by component from the free valence. At each step, when a choice is possible, the largest nomenclaturally significant component is chosen.

Contracted prefixes, such as methoxy are considered in their systematic uncontracted form, i.e. methyloxy.

Examples:

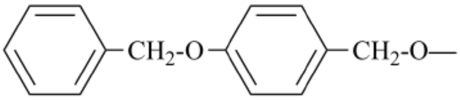
C_6H_5-CH_2-O–
benzyloxy (preferred prefix)
phenylmethoxy

Explanation: The primary component is ‘oxy’ in both prefixes (methoxy is treated as methyl and oxy). For the next component, there is a choice between ‘methyl’ and ‘benzyl’. ‘Benzyl’ is chosen; it is larger than ‘methyl’ leading to the prefix ‘benzyloxy’.



(4-chlorophenyl)methoxy (preferred prefix)
not (4-chlorobenzyl)oxy]

Explanation: The primary substituent is ‘oxy’ in both prefixes (‘methoxy’ is treated as ‘methyl’ and ‘oxy’). For the next component, there is a choice is between ‘methyl’ and a substituted ‘benzyl’. Since ‘benzyl’ is not substitutable, the alternative ‘methyl’ is the preferred secondary component, leading to ‘(phenylmethyl)oxy’ and finally to ‘(4-chlorophenyl)methoxy’.

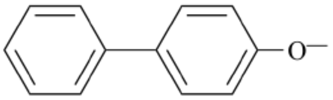


[4-(benzyloxy)phenyl]methoxy (prefered prefix)

Explanation: The primary substituent is ‘oxy’. As the ‘benzyl’ group that follows is substituted, the second component name, as shown in the second example above, is ‘phenylmethoxy’. The third component is ‘benzyloxy’ as described in the first example above, leading to the prefix ‘[(4-benzyloxy)phenyl]methoxy’.

C_6H_5-NH-CO-CH_2–
2-anilino-2-oxoethyl (preferred prefix)

Explanation: The primary component involves a choice between a ‘methyl’ group and a (substituted) ‘ethyl’ group. The larger ‘ethyl’ group is chosen. Then the choice for the second component is between ‘phenylamino’ and ‘anilino’; and ‘anilino’ is chosen as retained prefix preferred to ‘phenylamino’ (see P-62.2.1.1.1) leading to the prefix ‘2-anilino-2-oxoethyl’.



([1,1′-biphenyl]-4-yl)oxy (preferred prefix)
(not 4-phenylphenoxy)

Explanation: The primary component is 'oxy' ('phenoxy' is treated as 'phenyl' and 'oxy'). The next component is '[1,1′-biphenyl]-4-yl', derived from the preferred retained name '1,1′-biphenyl' (see P-29.3.5) which is larger than 'phenyl', which results in the prefix '([1,1′-biphenyl]-4-yl)oxy'.

$(CH_3)_2N\text{-}CO\text{-}NH\text{-}N=$
(dimethylcarbamoyl)hydrazinylidene (preferred prefix)
[not [(dimethylamino)carbonyl]hydrazinylidene]

Explanation: The primary component is 'hydrazinylidene' that is preferred to 'diazanylidene' (see P-68.3.1.2.1). The next component involves a choice between 'carbamoyl' and 'carbonyl'; 'carbamoyl' is larger and is preferred according to P-65.2.1.5. Thus, the preferred prefix is '(dimethylcarbamoyl)hydrazinylidene'.

$C_6H_{11}\text{-}CO\text{-}S\text{–}$
(cyclohexanecarbonyl)sulfanyl (preferred prefix)
[not (cyclohexylcarbonyl)sulfanyl]

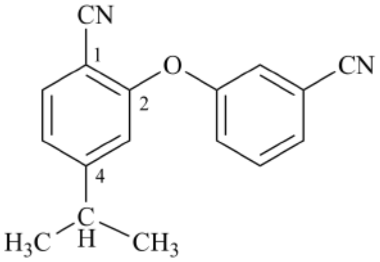
Explanation: The primary component is 'sulfanyl' in both prefixes. For the second component, the choice is between 'cyclohexanecarbonyl' and 'carbonyl'; 'cyclohexanecarbonyl' is larger and is preferred to the two-part prefix 'cyclohexylcarbonyl' (see P-65.1.7.4.2), resulting in the preferred prefix '(cyclohexanecarbonyl)sulfanyl'.

P-58 SELECTION OF PREFERRED IUPAC NAMES

P-58.1 INTRODUCTION.

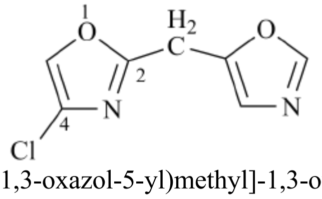
Section P-45 contains the hierarchical rules for choosing a preferred IUPAC name based on an order of seniority (see P-44) for determining the one and only parent structure. Preferred IUPAC names are generated under the condition that the name of the parent structure and the names of all or part of components are preferred IUPAC names. When this condition is not fulfilled and when the names of components are acceptable for general nomenclature, the resulting names of the compounds are acceptable only for general nomenclature.

Examples:



2-(3-cyanophenoxy)-4-(propan-2-yl)benzonitrile (PIN)
[not 3-[2-cyano-5-(propan-2-yl)phenoxy]benzonitrile;
the preferred IUPAC name has more substituents (see P-45.2.1)]

Explanation: The name 2-(3-cyanophenoxy)-4-isopropylbenzonitrile would also be acceptable in general nomenclature according to P-29.6.2.2)



4-chloro-2-[(1,3-oxazol-5-yl)methyl]-1,3-oxazole (PIN)
[not 2-[(4-chloro-1,3-oxazol-5-yl)methyl]-1,3-oxazole;
the preferred IUPAC name has more substituents (see P-45.2.1)]
4-chloro-2-[(oxazol-5-yl)methyl]oxazole (see P-22.2.1)

P-58.2 INDICATED HYDROGEN, 'ADDED INDICATED HYDROGEN', AND HYDRO PREFIXES

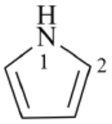
P-58.2.1 Indicated hydrogen (see also P-14.7.1).

Indicated hydrogen, if needed, is always cited at the front of the name of a spiro ring system, a bridged ring system, or a ring assembly, which is a change from its position in previous recommendations for bridged ring systems and ring assemblies where it was kept with the name of the individual ring.

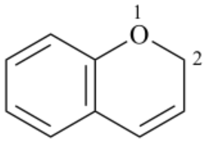
P-58.2.1.1 In many 'mancude' rings (see P-22.2.2.1.4), fused ring systems (see P-25.7.1.3), bridged fused ring systems (see P-25.7.1.3.3), spiro ring systems (see P-24.3), or ring assemblies (see P-28.2.3), it is necessary to specify hydrogen atoms of ring atoms that are attached only by single bonds to adjacent ring atoms in order that the principles of substitutive nomenclature can be used to describe characteristic groups, free valences, or ionic sites, i.e, to accommodate characteristic groups, free valences, or ionic sites. This is accomplished by specifying the presence of a hydrogen atom at such positions by the citation of an italicized capital '*H*' preceded by an appropriate numerical locant cited at the front of the name; this indicator is called 'indicated hydrogen'. Indicated hydrogen is often omitted for very common isomers or where there is no ambiguity in the name; however, in preferred IUPAC names indicated hydrogen must always be cited when present in the corresponding structure.

P-58.2.1.2 In parent hydrides, indicated hydrogen atoms (see P-14.7) are cited, if posible, at the lowest nonfusion peripheral atom (see P-25.0) of the ring or ring system consistent with the maximum number of noncumulative double bonds in accordance with P-25.7. Low locants are assigned to indicated hydrogen atoms when the degree of unsaturation is modified by using 'hydro' prefixes.

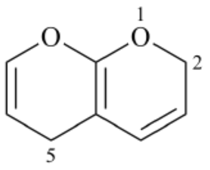
Examples:



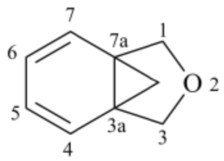
1*H*-pyrrole (PIN)



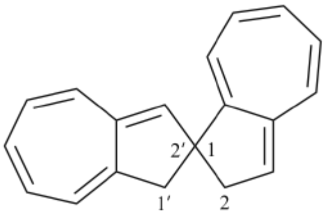
2*H*-1-benzopyran (PIN)



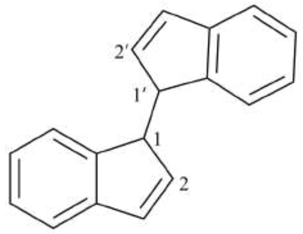
2*H*,5*H*-pyrano[2,3-*b*]pyran (PIN)



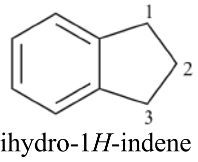
1*H*,3*H*-3a,7a-methano-2-benzofuran (PIN)



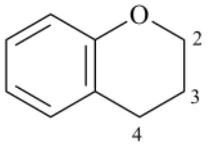
1′*H*,2*H*-1,2′-spirobi[azulene] (PIN)



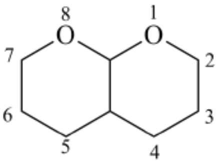
1*H*,1′*H*-1,1′-biindene (PIN)



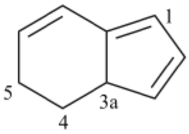
2,3-dihydro-1*H*-indene (PIN)
(not 1,3-dihydro-2*H*-indene;
nor 1,2-dihydro-3*H*-indene)



3,4-dihydro-2*H*-1-benzopyran (PIN)
(not 2,3-dihydro-4*H*-1-benzopyran;
although other indicated hydrogen combinations are possible,
this combination has the lowest possible locants that are structurally permissible for this compound)



58.2.1i
hexahydro-2*H*,5*H*-pyrano[2,3-*b*]pyran (PIN)



3a,5-dihydro-4*H*-indene (PIN)
(not 4,5-dihydro-3a*H*-indene)

P-58.2.2 'Added indicated hydrogen'

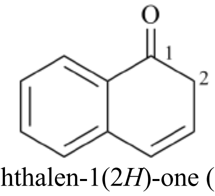
A second type of indicated hydrogen describes hydrogen atoms attached to ring atoms that are attached to adjacent ring atoms by single bonds only as the consequence of the addition of a suffix describing a structural modification. This type of indicated hydrogen is called 'added indicated hydrogen' because it is added to the name as a result of an operation on the parent hydride which may or may not contain indicated hydrogen atoms. 'Added indicated hydrogen' is cited in parentheses after the locant of the structural feature to which it refers. This method is preferred over the use of nondetachable hydro prefixes (P-58.2.5) for preferred IUPAC names.

Note: Indicated hydrogen has been used in the manner described in P-58.2.1, above but applied after the introduction of a principal characteristic group. It significantly reduced the need for 'added indicated hydrogen'. This method was developed at the Beilstein Institute and may be found in the *Beilsteins Handbuch der Organischen Chemie*, Springer Verlag, printed edition 1909-1959. It is not recommended for use in constructing IUPAC names but may be found in names in the literature.

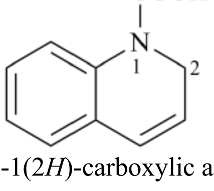
P-58.2.2.1 General methodology
The presence of at least one hydrogen atom on a ring atom that is attached to adjacent ring atoms by single bonds only that results from the introduction of a principal characteristic group, a free valence, radical, or an ionic center into a mancude polycyclic system in the absence of, or lack of, sufficient hydrogen atoms, is cited by using the capital italic letter *H* following the locant of the ring atom for each such position. This 'added indicated hydrogen' designation is enclosed in parentheses and inserted into the name immediately following the locant(s) for the free valences, radical or ionic centers, or principal characteristic groups.

P-58.2.2.2 When there is a choice, 'added indicated hydrogen' positions are assigned to periferal ring atoms, with the lowest locants consistent with the arrangement of double bonds in the compound as required. Low locants are assigned to 'added indicated hydrogen' atoms in the presence of hydro prefixes used to modify the degree of unsaturation.

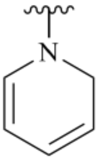
Examples:



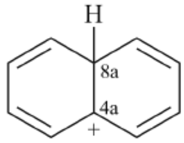
naphthalen-1(2*H*)-one (PIN)



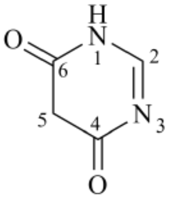
quinoline-1(2*H*)-carboxylic acid (PIN)



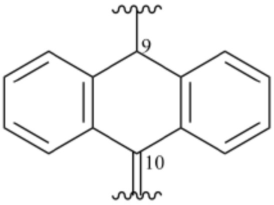
pyridin-1(2*H*)-yl (preferred prefix)



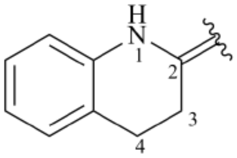
naphthalen-4a(8a*H*)-ylium (PIN)


H
N
1
2
O
6
5
4
N
3
O

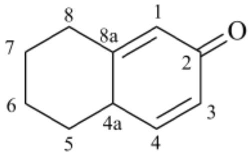
pyrimidine-4,6(1*H*,5*H*)-dione (PIN)



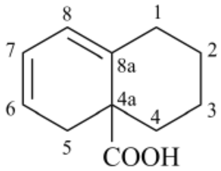
anthracen-9(10*H*)-yl-10-ylidene (preferred prefix)



3,4-dihydroquinolin-2(1*H*)-ylidene (preferred prefix)


8
1
O
7
8a
2
6
4a
3
5
4

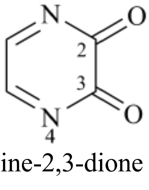
5,6,7,8-tetrahydronaphthalen-2(4a*H*)-one (PIN)


8
1
7
2
8a
4a
6
4
3
5
COOH

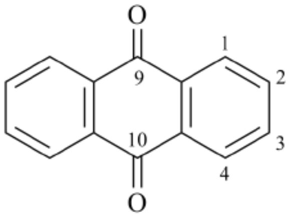
1,3,4,5-tetrahydronaphthalene-4a(2*H*)-carboxylic acid (PIN)
(a 4a(1*H*)-isomer is not consistent with the arrangement
of the double bonds in the mancude compound)

P-58.2.2.3 'Added indicated hydrogen' atoms are not cited when the accommodation of a pair of principal characteristic groups or free valences simply removes a double bond (directly or after rearrangement of double bonds) from the parent ring structure.

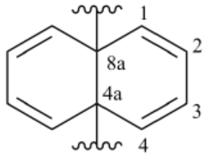
Examples:



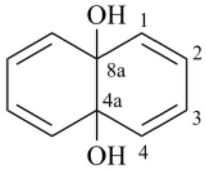
pyrazine-2,3-dione (PIN)



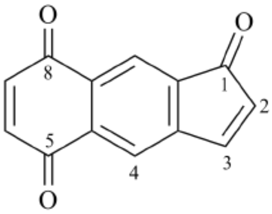
anthracene-9,10-dione (PIN)



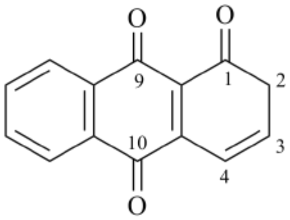
naphthalene-4a,8a-diyl (preferred prefix)



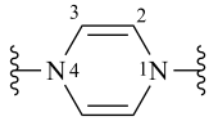
naphthalene-4a,8a-diol (PIN)



1*H*-cyclopenta[*b*]naphthalene-1,5,8-trione (PIN)



anthracene-1,9,10(2*H*)-trione (PIN)



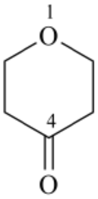
pyrazine-1,4-diyl (preferred prefix)

P-58.2.3 Specific rules related to indicated hydrogen, 'added indicated hydrogen' and hydro prefixes

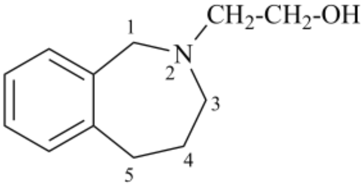
P-58.2.3.1 Indicated hydrogen is cited at any position of a ring system in order to accommodate principal characteristic groups or free valences expressed as suffixes, provided that there are an equal or greater number of indicated hydrogen atoms available to accommodate all of the principal characteristic groups or free valences.

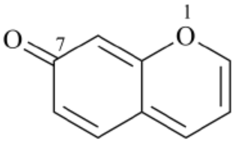
P-58.2.3.1.1 When there are an equal number of indicated hydrogen atoms and principal characteristic groups or free valences to be accommodated, the indicated hydrogen atoms are placed at peripheral atoms that will accommodate these principal characteristic groups or free valences. Locants for hydro prefixes are those of the saturated positions.

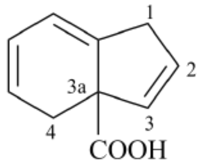
Examples:

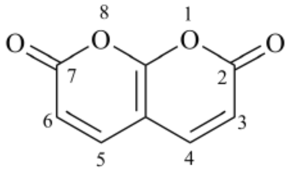


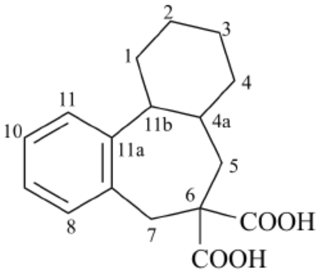
tetrahydro-4*H*-pyran-4-one
oxan-4-one (PIN)

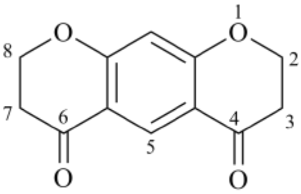

2-(1,3,4,5-tetrahydro-2*H*-2-benzazepin-2-yl)ethan-1-ol (PIN)
1,3,4,5-tetrahydro-2*H*-2-benzazepine-2-ethanol

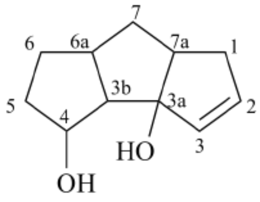

7*H*-1-benzopyran-7-one (PIN)

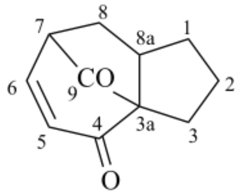

1,4-dihydro-3a*H*-indene-3a-carboxylic acid (PIN)


2*H*,7*H*-pyrano[2,3-*b*]pyran-2,7-dione (PIN)


1,2,3,4,4a,5,7,11b-octahydro-6*H*-dibenzo[*a*,*c*][7]annulene-6,6-dicarboxylic acid (PIN)
[not 1,2,3,4,4a,5,7,11b-octahydro-6*H*-dibenzo[*a*,*c*]cycloheptene-6,6-dicarboxylic acid]

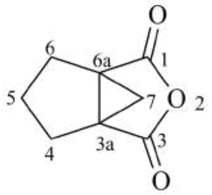

2,3,7,8-tetrahydro-4*H*,6*H*-benzo[1,2-*b*:5,4-*b*′]dipyran-4,6-dione (PIN)


1,3b,4,5,6,6a,7,7a-octahydro-3a*H*-cyclopenta[*a*]pentalene-3a,4-diol (PIN)

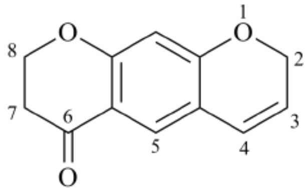

1,2,3,7,8,8a-hexahydro-4*H*-3a,7-methanoazulene-4,9-dione (PIN)

P-58.2.3.1.2 When there are more indicated hydrogen atoms than can be used to accommodate all of the principal characteristic groups or free valences in the structure of the compound, the remaining indicated hydrogen atoms are assigned to the lowest nonfusion peripheral atom consistent with the arrangement of double bonds in the compound. Locants for ‘hydro’ prefixes are those of the saturated positions.

Examples:



5,6-dihydro-1*H*,3*H*,4*H*-3a,6a-methanocyclopenta[*c*]furan-1,3-dione (PIN)
(not 4,5-dihydro-1*H*,3*H*,6*H*-3a,6a-methanocyclopenta[*c*]furan-1,3-dione;
4*H* is lower than 6*H*)



7,8-dihydro-2*H*,6*H*-benzo[1,2-*b*:5,4-*b*′]dipyran-6-one (PIN)
(not 2,3-dihydro-4*H*,8*H*-benzo[1,2-*b*:5,4-*b*′]dipyran-4-one;
‘2*H*,6*H*’ is lower than ‘4*H*,8*H*’)
(not 6,7-dihydro-2*H*,8*H*-benzo[1,2-*b*:5,4-*b*′]dipyran-4(3*H*)-one;
‘2*H*,6*H*’ is lower than ‘2*H*,8*H*’)

P-58.2.3.1.3 When the number of indicated hydrogens is less than the number of characteristic groups the following rules are applied.

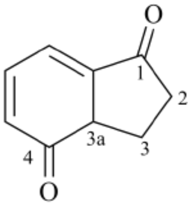
(1) at least one of the indicated hydrogen atoms is assigned to a nonfusion peripheral atom having the lowest locants consistent with the mancude system of double bonds as established in P-58.2.1.2.

(2) other indicated hydrogen atoms are assigned to other positions that accommodate characteristic groups or free valences.

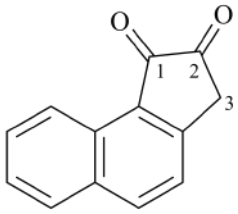
(3) principal characteristic groups or free valences that cannot be accommodated in ways described in (1) and (2) are accommodated by using ‘added indicated hydrogen atoms’ (see P-58.2.2).

(4) indicated hydrogen atoms that cannot be used to accommodate principal characteristic groups or free valences has seniority over ‘added indicated hydrogen’ for lower locants.

Examples:

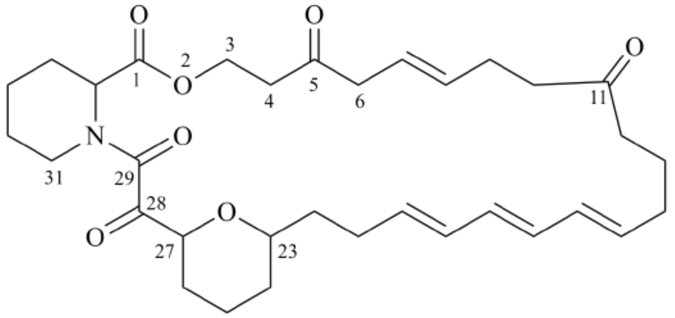


3,3a-dihydro-1*H*-indene-1,4(2*H*)-dione (PIN)



1*H*-cyclopenta[*a*]naphthalene-1,2(3*H*)-dione (PIN)
(not 3*H*-cyclopenta[*a*]naphthalene-1,2-dione)

Explanation: There is only one indicated hydrogen atom but there are two principal characteristic groups to be accommodated; therefore the indicated hydrogen is placed at the lowest position consistent with the arrangement of the double bonds in the parent ring system.

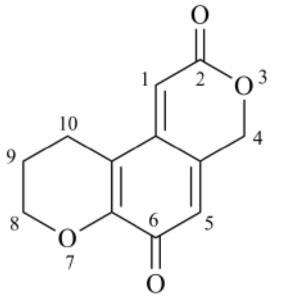


9,10,12,13,14,21,22,23,24,25,26,27,32,33,34,34a-hexadecahydro-3*H*-23,27-epoxypyrido[2,1-*c*][1,4]oxaazacyclohentriacontine-1,5,11,28,29(4*H*,6*H*,31*H*)-pentone (PIN)

Explanation: The ring system requires only one indicated hydrogen atom but there are 5 ketonic sites, the principal characteristic groups; thus, the indicated hydrogen atom is assigned to position 3, the lowest possible site consistent with the arrangement of the double bonds in the compound (position 1 is not possible because of the fused pyrido ring). The ketonic sites 28 and 29 simply remove a double bond from the fused ring system and do not require added hydrogen atoms. The ketonic sites at 1, 5, and 11 remain to be accommodated. As noted above, because of the fused pyrido ring there must be an 'added indicated hydrogen' atom the fused pyrido ring and it must be at lowest position, 31. Finally, added indicated hydrogen atoms are inserted at the lowest positions consistent with the arrangement of the double bonds in the compound to accommodate the ketonic sites at 5 and 11, and the appropriate number of hydro prefixes added.

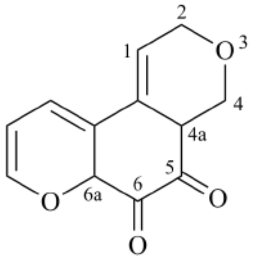
P-58.2.3.1.4 When the indicated hydrogen atoms of a parent structure cannot be used to accommodate all of the principal characteristic groups of the structure, the rules described in P-58.2.3.1.3 are applied.

Examples:



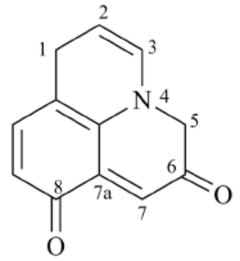
9,10-dihydro-2*H*,4*H*-benzo[1,2-*b*:4,3-*c*′]dipyran-2,6(8*H*)-dione (PIN)

Explanation: The indicated hydrogen atoms cannot accommodate both '-one' principal characteristic group positions, (2*H*,6*H*-benzo[1,2-*b*:4,3-*c*′]dipyran is not a permissible structure) so the indicated hydrogen atoms and the necessary 'added indicated hydrogen' atom are placed at the lowest locant positions consistent with the arrangement of the double bonds in the compound.



4,4a-dihydro-2*H*,5*H*-benzo[1,2-*b*:4,3-*c*′]dipyran-5,6(6a*H*)-dione (PIN)
(not 4,4a-dihydro-2*H*,4*H*-benzo[1,2-*b*:4,3-*c*′]dipyran-5,6(4a*H*,6a*H*)-dione)

Explanation: The indicated hydrogen atoms cannot accommodate both '-one' principal characteristic group positions; therefore one indicted hydrogen atom is assigned at the lowest locant position; the second indicated hydrogen atom is assigned to position '5' to accommodate one of the 'one' principal characteristic groups.



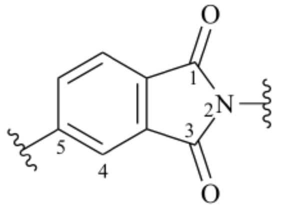
1*H*,5*H*-pyrido[3,2,1-*ij*]quinoline-6,8-dione (PIN)

Explanation: The indicated hydrogen atoms cannot accommodate either of the ‘one’ principal characteristic group positions; (6*H*,8*H*-pyrido[3,2,1-*ij*]quinoline is not a permissible structure), so the indicated hydrogen atoms are placed at the lowest locant positions consistent with the arrangement of the double bonds in the compound; no ‘added indicated hydrogen’ is necessary since the two ‘-one’ principal characteristic groups simply remove one double bond from the parent structure.

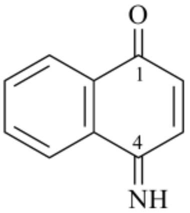
P-58.2.4 Prefix nomenclature

After the introduction of indicated and ‘added indicated hydrogen’ atoms, all substituent groups not expressed as suffixes are cited as prefixes.

Examples:



1,3-dioxo-1,3-dihydro-2*H*-isoindole-2,5-diyl (preferred prefix)



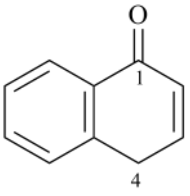
4-iminonaphthalen-1(4*H*)-one (PIN)

P-58.2.5 Nondetachable hydro prefixes *vs*. indicated hydrogen

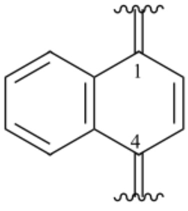
An alternative method to the ‘added indicated hydrogen’ method for accommodation of principal characteristic groups, free valences, radicals, or ionic centers at positions of mancude parent hydrides where a sufficient number of hydrogen atoms for the operation of the basic principles of substitutive nomenclature are not present is to derive them from a suitable hydrogenated derivative of the parent ring system.

Rule C-16.11 in the 1979 edition of the *IUPAC Nomenclature of Organic Chemistry* (ref. 1) allows for hydro prefixes to be either nondetachable, i.e., they must always be cited directly in front of the name of a fully unsaturated parent structure, thus creating a parent hydride separate and distinct from the fully unsaturated analogue, or detachable, i.e., cited as prefixes in front of the name of a fully unsaturated parent structure, but alphabetized among any substituent prefixes that may also be present. The 1993 Guide (ref. 1) formalized the nondetachable method. In these recommendations, the use of nondetachable hydro prefixes is not used in preferred IUPAC names, but may be used in general nomenclature. This method often leads to differences in numbering of the parent structure (see fourth example, below).

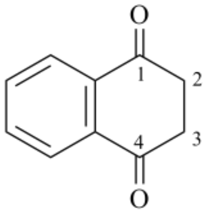
Examples:



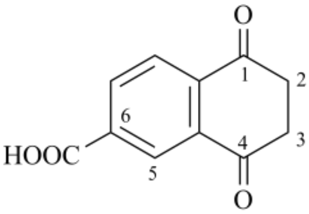
1,4-dihydronaphthalen-1-one
naphthalen-1(4*H*)-one (PIN)



1,4-dihydronaphthalene-1,4-diylidene
naphthalene-1,4-diylidene (preferred prefix;
see P-58.2.2.3)



1,2,3,4-tetrahydronaphthalene-1,4-dione
2,3-dihydronaphthalene-1,4-dione (PIN;
see P-58.2.2.3)



1,4-dioxo-1,2,3,4-tetrahydronaphthalene-6-carboxylic acid
(numbering shown; nondetachable hydro prefixes are part of the parent hydride
and have precedence over the principal characteristic group for low numbering)
5,8-dioxo-5,6,7,8-tetrahydronaphthalene-2-carboxylic acid (PIN)
(detachable but nonalphabetized hydro prefixes do not have precedence
over the principal characteristic group for low numbering,
but has precedence over other detachable prefixes).

P-58.3 HOMOGENEOUS HETERO CHAINS AND FUNCTIONAL GROUPS

P-58.3.1 Preselected names for unbranched homogeneous heteroacyclic parent hydrides other than boron hydrides are described in P-21.2.2. Potential functionality of terminal groups, such as $-NH_2$, –SH, or –OH, attached to parent chains of the same heteroatom are ignored; they simply extend the chain. For boron chains see P-68.1.1.2. For chains involving chalcogen atoms, see P-68.4.

P-58.3.2 When one or more atoms of a homogeneous heteroatomic chain can be expressed by a principal characteristic group, a functional parent compound, or a compulsory prefix, the principal characteristic group or compulsory prefix group is expressed. Hence, an acyclic homogeneous heterocyclic chain may be broken in order to recognize a senior function as a principle characteristic groups, functional parent compound, or compulsory prefix.

Examples:

$HS\text{-}SO_2\text{-}S\text{-}S\text{-}S\text{-}SO_2\text{-}SH$
trisulfanedisulfonothioic *S*-acid (preselected name)
(not heptasulfane-2,2,6,6-tetrone)

$H_2N\text{-}NH\text{-}NH\text{-}NH\text{-}CO\text{-}C_6H_5$
N-(triazan-1-yl)benzamide (PIN)
[not phenyl(tetraazan-1-yl)methanone;
nor 1-benzoyltetraazane]

$H_2N\text{-}NH\text{-}NH\text{-}NH\text{-}COOH$
tetraazane-1-carboxylic acid (PIN)
[not (triazan-1-yl)carbamic acid;
the carboxylic acid is senior to the carbonic acid derivative]

$CH_3\text{-}NH\text{-}N(COOH)\text{-}NH\text{-}CH_3$
1,3-dimethyltriazane-2-carboxylic acid (PIN)
(not bis(methylamino)carbamic acid;
the carboxylic acid is senior to the carbonic acid derivative)

$(CH_3)_2P\text{-}P(OH)\text{-}P(CH_3)_2$
bis(dimethylphosphanyl)phosphinous acid (PIN)
(not 1,1,3,3-tetramethyltriphosphan-2-ol)

$H_2N\text{-}NO$
nitrous amide (preselected name)
(not hydrazinone; (see P-61.6)

$H_2N\text{-}NH\text{-}NH\text{-}NCO$
1-isocyanatotriazane (PIN)
[not 1-(oxomethylidene)tetraazane]

$C_6H_5\text{-}CO\text{-}NH\text{-}NH\text{-}NH\text{-}NH\text{-}CO\text{-}C_6H_5$
N,*N*′-(hydrazine-1,2-diyl)dibenzamide (PIN)

$OCN\text{-}NH\text{-}NO_2$
isocyanatonitramide (PIN)

$HS\text{-}S\text{-}S\text{-}S\text{-}CO\text{-}C_6H_5$
phenyl(tetrasulfanyl)methanone (PIN)
[not trisulfanyl benzenecarbothioate;
pseudoesters are not recognized when the alcoholic component
is a chalcogen atom (see P-65.6.3.4.2 and P-68.4.2.4)]

P-59 NAME CONSTRUCTION

P-59.0 Introduction
P-59.1 General methodology
P-59.2 Examples illustrating the methodology

P-59.0 INTRODUCTION

This Section describes the procedure for the systematic formation of a preferred IUPAC name for an organic compound. This procedure can also be followed for generation of names for general nomenclature.

P-59.1 GENERAL METHODOLOGY

The procedure for formation of a preferred systematic name for an organic compound involves a number of steps outlined in this and in the following subsections, to be taken as far as they are applicable in the following order.

P-59.1.1 From the nature of the compound, determine the type(s) of nomenclature (see P-15) and operations (see P-13) to be used. Although the type of nomenclature called ‘substitutive nomenclature’ (see P-15.1) is the preferred type of nomenclature for generating preferred IUPAC names and for general nomenclature, other nomenclature types must be used when specified by specific classes of compounds rules:

(1) ‘functional class nomenclature’, for compounds such as esters and acid halides (see P-15.2 and P-51.2 for preferred IUPAC names and for general nomenclature);

(2) ‘multiplicative nomenclature’ (see P-15.3, and P-51.3 for preferred IUPAC names and for general nomenclature);

(3) ‘skeletal replacement (‘a’) nomenclature’ (see P-15.4 and P-51.4 for preferred IUPAC names and for general nomenclature).

When configurations are expressed in the structure, select the type of nomenclature, substitutive or multiplicative nomenclature according to P-93.6, that will take them into consideration.

P-59.1.2 Determine the class to which the compound belongs and the characteristic group to be cited as the suffix as given in P-33, (if any) in accord with the seniority order of classes as indicated in P-41 or as a functional class name (see P-15.2). Only one kind of characteristic group (known as the principal group) can be cited as suffix or functional class name.

Suffixes listed in P-33 are used to generate both preferred IUPAC names and names in general nomenclature. The order of seniority of suffixes discussed in P-43 is mandatory for constructing preferred IUPAC names and in general nomenclature. All atoms or groups not so cited must be specified as substituent prefixes.

Radicals and ions are named using suffixes that have the unique property of being cumulative, both among themselves and in conjunction with certain suffixes that express characteristic groups (see Chapter P-7 for seniority order of radicals and ions to be used to generate preferred IUPAC names and in general nomenclature).

P-59.1.3 Select the parent hydride(s), including any appropriate nondetachable prefixes as described in Chapter P-2 and in P-52 for the selection of preferred IUPAC names, or functional parent compound as described in P-34 for preferred IUPAC names and in Chapter P-6 for various classes such as amines, alcohols, etc. which summarizes two aspects of the use of functional parent compounds in substitutive nomenclature, i.e., use as preferred IUPAC name or in general nomenclature and their substitutability. Determine the senior parent structure, either in the presence of a suffix describing the principal characteristic group or in the absence of any such suffix. All required descriptors for indicating changes from standard bonding number and isotopic modifications must be introduced at this stage.

P-59.1.4 Name the parent hydride, as described in P-59.1.3 and the principal characteristic group, if any, according to P-33, or the functional parent compound according to P-34 and Chapter P-6, using rules indicated in P-43 in order to take functional modifications into consideration. For ketones and imines, use Rules discussed in P-58.2 for generating preferred IUPAC names and for general nomenclature.

P-59.1.5 Determine suffixes and/or prefixes, in accordance with P-15.5, P-57, Chapter P-6, and Appendix 2 using appropriate multiplying prefixes (see P-14.2) and number the parent structure as far as possible using the general rule P-14.4.

P-59.1.6 Name substituent groups and characteristic groups not cited as principal characteristic groups as prefixes (alphabetized prefixes) in accordance with P-34 which summarizes the use of functional parent compounds in substitutive nomenclature, i.e., use as preferred IUPAC name or in general nomenclature, and P-15.1.8 for their substitutability and P-56 for preferred IUPAC names and for allowed names in general nomenclature, and complete the numbering of the structure, if necessary, according to the numbering rules for nomenclatural features given in P-14.4.

P-59.1.7 Assemble the components into a complete name, using rules described in Section P-14 (general rules) related to locants, numbering, alphanumerical order, indicated and added indicated hydrogen and aspects of name writing such as punctuation, enclosing marks, italicization, elision and addition of vowels, and primes as described in P-16.

P-59.1.8 Complete the name with all required descriptors for stereochemical features in accordance with rules described in Chapter P-9.

P-59.1.9 Characteristic groups

In substitutive nomenclature, some characteristic groups can be denoted either as suffixes or prefixes (see P-33 and P-35), but others only as prefixes (see Table 5.1). Functional class names differ in that a separate word (or a suffix in some languages) designating the name of a functional class is associated with a substituent group name describing the reminder of the structure.

Characteristic groups that can be cited as suffixes in substitutive nomenclature are not necessarily identical with groups designated by the name of a corresponding functional class when functional class names are formed (e.g., butanone and ethyl methyl ketone, where ‘one’ denotes =O and ‘ketone’ denotes –CO–).

The characteristic groups listed in Table 5.1 are always cited as prefixes to the name of the parent structure described in Chapter P-2. Multiplying prefixes (see P-14.2) and locants are added as necessary (see P-14.3).

Table 5.1 Characteristic groups always cited as prefixes in substitutive nomenclature

Characteristic group	Prefix	Characteristic group	Prefix
–Br	bromo	–IO[1]	iodosyl
–BrO[1]	bromosyl	–IO_2[1]	iodyl
–BrO_2[1]	bromyl	–IO_3[1]	periodyl
–BrO_3[1]	perbromyl	–O-R[2,3]	alkoxy
–Cl	chloro	–O-O-R[2,4]	alkylperoxy
–ClO[1]	chlorosyl	=N_2	diazo
–ClO_2[1]	chloryl	–N_3	azido
–ClO_3[1]	perchloryl	–NCO[5]	isocyanato
–F	fluoro	–NC	isocyano
–FO[1]	fluorosyl	–NO[1]	nitroso
–FO_2[1]	fluoryl	–NO_2[1]	nitro
–FO_3[1]	perfluoryl	–S(O)-R[2,6]	alkanesulfinyl
–I	iodo	–$S(O)_2$-R[2,6]	alkanesulfonyl

[1] And also chalcogen analogs, as thiochlorosyl, selenochloryl, dithiochloryl, and thionitroso.

[2] ‘R’ designates an ‘organic’ substituent group, as methoxy, pentyloxy, phenylperoxy, methanesulfonyl or methylsulfinyl, and benzenesulfonyl or phenylsulfonyl.

[3] Also included are chalcogen analogues, such as alkyl- or arylsulfanyl, alkyl- or arylselanyl, and alkyl- or aryltellanyl.

[4] Also included are chalcogen analogues, as methoxysulfanyl, methylsulfanyloxy, and methyldisulfanyl.

[5] Also included are chalcogen analogues, as isothiocyanato and isoselenocyanato.

[6] Includes selenium and tellurium analogues and all chalcogen analogues, as methanesulfinothioyl and benzeneselenotelluronyl.

Examples:

$$\mathrm{Cl\text{-}\overset{1}{C}H_2\text{-}\overset{2}{C}H_2\text{-}\overset{3}{C}H_2\text{-}Cl}$$

1,3-dichloropropane (PIN)

$C_6H_5\text{-}NO$

nitrosobenzene (PIN)

Characteristic groups other than those listed in Table 5.1 may be cited as either suffixes or prefixes to the name of the parent hydride.

If characteristic groups other than those given in Table 5.1 are present, one (and only one) kind must be cited as suffix (the principal characteristic group) for classes other than radicals and ions.

When a compound contains more than one kind of characteristic group not given in Table 5.1, the principal characteristic group is the one that characterizes the class occurring earliest (i.e., nearest to the top) in the seniority order of classes (see P-41, P-42 and P-43, if necessary). All other characteristic groups are cited as prefixes.

If, and only if, the complete suffix (that is, the suffix plus its multiplying prefixes, if any) begins with a vowel, a terminal letter ‘e’ (if any) of the parent hydride name is elided. For example, ethanol (not ethaneol). Elision or retention of the terminal letter ‘e’ is independent of the presence of numerals between it and the following letter, for example, propan-2-ol (not propane-2-ol).

When a substituent is itself substituted (compound substituent, see P-29.4, P-35.3 and P-46), all the subsidiary substituents are named as prefixes. The substituent bearing the subsidiary substituent is regarded as a parent substituent (analogous to a parent hydride). The nomenclature of the whole substituent is subject to all the procedures adopted for compounds, with two exceptions, which are:

(a) that no characteristic group is expressed as a suffix (instead, a suffix such as ‘yl’, ‘ylidene’, etc., is used); and

(b) that the point of attachment of the substituent has the lowest permissible locant.

P-59.1.10 Numbering nomenclatural features

When the parent hydride (principal chain, ring, or ring system), principal group and substituents have been selected and named, the numbering of the complete compound is allocated using the rule of lowest locants. General rules for locants and numbering are described in P-14.4. They do apply each and every time a name is constructed, not only for substitutive and functional class nomenclature, but for all types of nomenclature.

The list of seniority of structural features that receive lowest possible locants has been refined by reallocating the placement of the ‘a’ prefixes for skeletal replacement (‘a’) nomenclature in chains and by giving a special status of detachable prefix to hydro/dehydro prefixes.

Insofar as the preceding rules leave a choice, the starting point and direction of numbering of a compound are chosen so as to give lowest locants to the structural features (if present) considered successively in the order given until a decision is reached:

(a) fixed numbering, as for naphthalene, bicyclo[2.2.2]octane, etc.;

(b) heteroatoms in heterocycles and in acyclic parent structures;

(c) indicated hydrogen [for unsubstituted compounds; a higher locant may be needed at another position to provide for a substituent suffix in accordance with structural feature (d)];

(d) principal group named as suffix;

(e) ‘added indicated hydrogen’ (consistent with the structure of the compound and in accordance with further substitution);

(f) saturation (‘hydro’/‘dehydro’ prefixes) or unsaturation (‘ene’/‘yne’ endings);

(g) substituents named as prefixes (low locants are allocated for substituents regardless of kind; then, if necessary, in the order of citation in the name).

P-59.2 EXAMPLES ILLUSTRATING THE GENERAL METHODOLOGY

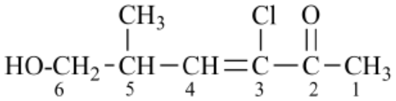
P-59.2.1 Selection of parent hydrides
P-59.2.2 Seniority of heteroatoms over suffixes
P-59.2.3 Seniority of principal characteristic groups over unsaturation
P-59.2.4 Seniority of 'ene' and 'yne' endings and hydro prefixes over detachable prefixes
P-59.2.5 Treatment of detachable prefixes

P-59.2.1 Selection of parent compounds

After the principal characteristic group has been chosen and named, the parent hydride or functional parent compound is chosen by one of the following methods. For details of numbering, see Chapter P-2 describing the numbering of the various parent hydrides and the general rule of lowest locants as formulated in P-14.3. For the arrangement of prefixes, see the general rule on alphanumerical order described in P-14.5.

P-59.2.1.1 If the compound is purely acyclic, the principal chain is chosen as parent hydride by the method described in P-44.

Example:



$$\underset{6}{\mathrm{HO\text{-}CH_2}}\text{-}\underset{5}{\overset{\mathrm{CH_3}}{\overset{|}{\mathrm{CH}}}}-\underset{4}{\mathrm{CH}}=\underset{3}{\overset{\mathrm{Cl}}{\overset{|}{\mathrm{C}}}}-\underset{2}{\overset{\mathrm{O}}{\overset{\|}{\mathrm{C}}}}-\underset{1}{\mathrm{CH_3}}$$

Analysis

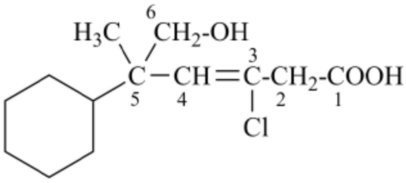
Principal group:	>C=O	one
Parent hydride:	CH_3-CH_2-CH_2-CH_2-CH_2-CH_3	hexane
Functionalized parent hydride	CH_3-CH_2-CH_2-CH_2-CO-CH_3	hexan-2-one
Subtractive modification	CH_3-CH_2-CH=CH-CO-CH_3	hex-3-en-2-one
Substituents:	–Cl	chloro
	–OH	hydroxy
	–CH_3	methyl

Together with other rules, this analysis leads to the preferred IUPAC name:
3-chloro-6-hydroxy-5-methylhex-3-en-2-one (PIN)

Explanation: The suffix 'one' receives the lowest possible locant, '2', thus determining the direction of numbering of the chain. Two hexane chains are possible; the principal chain, in accord with the criteria for selecting the principal chain, is the one that is most substituted (3 substituents compared to 2). Unsaturation is denoted by the ending 'ene'. The three substituent prefixes are arranged in alphanumerical order to complete the name.

P-59.2.1.2 If the principal group occurs only in a chain that carries a substituent, the compound is named as an acyclic compound and cyclic component is expressed by a substituent prefix.

Example:



Analysis

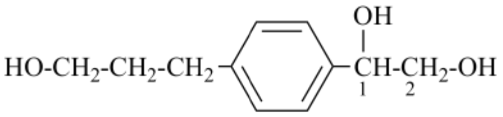
Principal group:	(C)OOH	oic acid
Parent hydride:	CH_3-CH_2-CH_2-CH_2-CH_2-CH_3	hexane
Functionalized parent hydride	CH_3-CH_2-CH_2-CH_2-CH_2-COOH	hexanoic acid
Subtractive modification	CH_3-CH_2-CH=CH-CH_2-COOH	hex-3-enoic acid
Substituents:	Cl–	chloro
	C_6H_{11}–	cyclohexyl
	HO–	hydroxy
	CH_3–	methyl

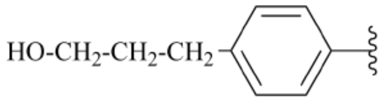
Together with other rules, this analysis leads to the preferred IUPAC name:
3-chloro-5-cyclohexyl-6-hydroxy-5-methylhex-3-enoic acid (PIN)

Explanation: The presence of a carboxylic acid group at the end of the chain determines the direction of its numbering. The 'ene' ending and the substituent prefixes, in alphanumerical order, are located on the chain in accord with its determined numbering.

P-59.2.1.3 If the principal group occurs in two or more carbon chains that are not attached to one another (that is, do not together form a continuous or branched chain but are separated by, for instance, a ring or a heteroatom), and when multiplicative nomenclature is not possible, then the chain carrying the largest number of the principal groups is chosen as the parent hydride for nomenclature; if the numbers of these groups in two or more chains are the same, choice is made by the principles for selection of the principal chain.

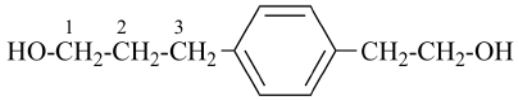
Example 1:

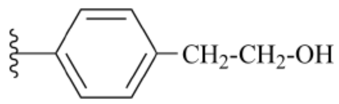


Analysis		
Principal group:	OH	diol
Parent hydride:	CH_3-CH_3	ethane
Functionalized parent hydride	HO-CH_2-CH_2-OH	ethane-1,2-diol
Substituent:		
Substituent components:	OH –CH_2-CH_2-CH_3 –C_6H_5	hydroxy propyl phenyl
Substituent prefix:	4-(3-hydroxypropyl)phenyl	

Together with other rules, this analysis leads to the preferred IUPAC name:
1-[4-(3-hydroxypropyl)phenyl]ethane-1,2-diol (PIN)

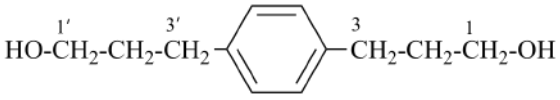
Example 2: In the following example, the longest chain is chosen as parent hydride, in accord with the criteria for selecting the principal chain.

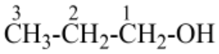


Analysis		
Principal group:	–OH	ol
Parent hydride:	CH_3-CH_2-CH_3	propane
Functionalized parent hydride	CH_3-CH_2-CH_2-OH	propan-1-ol
Substituent:		
Substituent components:	–OH –CH_2-CH_3 –C_6H_5	hydroxy ethyl phenyl
Substituent prefix:	4-(2-hydroxyethyl)phenyl	

Together with other rules, this analysis leads to the preferred IUPAC name:
3-[4-(2-hydroxyethyl)phenyl]propan-1-ol (PIN)

Example 3:



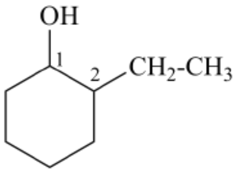
Analysis		
Principal group:	OH	ol
Parent hydride:	CH_3-CH_2-CH_3	propane
Functionalized parent hydride	 $\overset{3}{C}H_3\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}H_2\text{-}OH$	propan-1-ol
Multiplicativ connecting group:	–C_6H_5–	1,4-phenylene

Together with other rules, this analysis leads to the preferred IUPAC name:
3,3′-(1,4-phenylene)di(propan-1-ol) (PIN)

Explanation: A multiplicative name is formed when identical parent structures are attached symmetrically to a central component (for a preferred IUPAC name the parent structures must be symmetrically substituted). The numbering of the multiplied parent structure, which includes the characteristic group, if any, is retained.

P-59.2.1.4 If the principal group occurs only in a single cyclic system, that cyclic system is chosen as parent hydride for nomenclature.

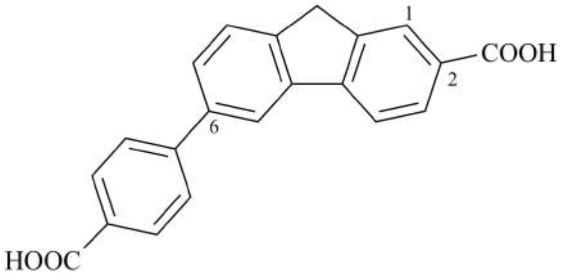
Example:

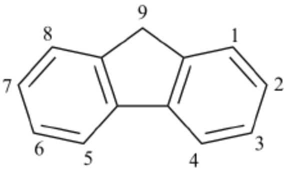
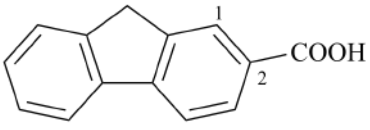


Analysis		
Principal group:	–OH	ol
Parent hydride:	C_6H_{12}	cyclohexane
Functionalized parent hydride	C_6H_{11}-OH	cyclohexanol
Substituent:	–CH_2-CH_3	ethyl

Together with other rules, this analysis leads to the preferred IUPAC name:
2-ethylcyclohexan-1-ol (PIN)

P-59.2.1.5 If the principal group occurs in more than one cyclic system, the cyclic system chosen as parent hydride for nomenclature is in accordance with the criteria for choosing a senior ring or ring system.

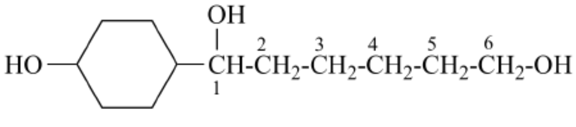


Analysis		
Principal group:	–COOH	carboxylic acid
Parent hydride:		9*H*-fluorene
Functionalized parent hydride		9*H*-fluorene-2-carboxylic acid
Substituents:	–C_6H_5	phenyl
	–COOH	carboxy

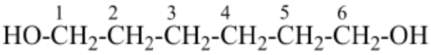
Together with other rules, this analysis leads to the preferred IUPAC name:
6-(4-carboxyphenyl)-9*H*-fluorene-2-carboxylic acid (PIN)

P-59.2.1.6 If the principal group occurs both in a chain and in a cyclic system, the parent hydride for nomenclature is the portion in which the principal group occurs in the greater number; if the number of occurrences of the principal group is the same in two or more portions, the ring or ring system is chosen as parent hydride for nomenclature.

Example 1:

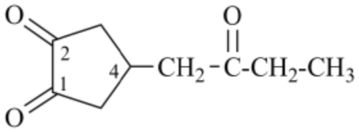


Analysis		
Principal group:	–OH	diol

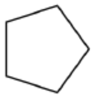
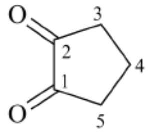
Parent hydride:	CH_3-CH_2-CH_2-CH_2-CH_2-CH_3	hexane
Functionalized parent hydride	 $\overset{1}{\text{HO-CH}_2}\text{-}\overset{2}{\text{CH}_2}\text{-}\overset{3}{\text{CH}_2}\text{-}\overset{4}{\text{CH}_2}\text{-}\overset{5}{\text{CH}_2}\text{-}\overset{6}{\text{CH}_2}\text{-OH}$	hexane-1,6-diol
Substituent components:	–C_6H_{11}	cyclohexyl
	–OH	hydroxy
Substituent prefix:	4-hydroxycyclohexyl	

Together with other rules, this analysis leads to the preferred IUPAC name:
1-(4-hydroxycyclohexyl)hexane-1,6-diol (PIN)

Example 2:



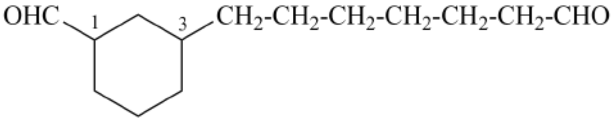
Analysis

Principal group:	(C)O	dione
Parent hydride:		cyclopentane
Functionalized parent hydride		cyclopentane-1,2-dione
Substituents:	=O	oxo
	CH_3-CH_2-CH_2-CH_2–	butyl
Substituent prefix:	2-oxobutyl	

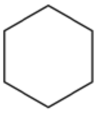
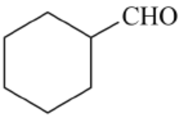
Together with other rules, this analysis leads to the preferred IUPAC name:
4-(2-oxobutyl)cyclopentane-1,2-dione (PIN)

P-59.2.1.7 If the number of occurrences of the principal group is the same in two or more nomenclaturally significant parts of the compound, preferred IUPAC names are formed by choosing the ring or ring system as parent hydride for nomenclature.

Example:



Analysis

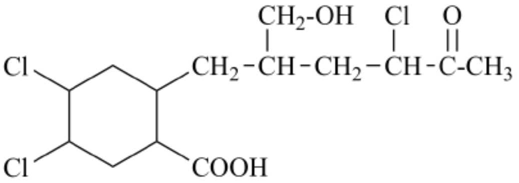
Principal group:	–CHO	carbaldehyde
Parent hydride:		cyclohexane
Functionalized parent hydride		cyclohexanecarbaldehyde
Substituent:	–CH_2-$[CH_2]_5$-CHO	7-oxoheptyl

Together with other rules, this analysis leads to the preferred IUPAC name:
3-(7-oxoheptyl)cyclohexane-1-carbaldehyde (PIN)

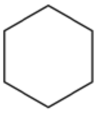
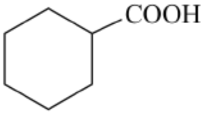
In general nomenclature, a chain may be chosen as the parent hydride, depending on the importance given to a specific portion (Rule P-44.1.2.2), leading to the name: 7-(3-formylcyclohexyl)heptanal

P-59.2.1.8 When a substituent is itself substituted, all the subsidiary substituents are named as prefixes. The substituent bearing the subsidiary substituents is regarded as a 'parent substituent' (analogous to a parent compound). The nomenclature of the whole substituent is subject to all the procedures adopted for compounds (for instance, choice of principal chain), with two exceptions, namely: (a) that no suffix is used, and (b) that the point of attachment of the substituent bears the lowest permissible locant number depending on the nomenclature of the substituent group, alkyl or alkanyl.

Example:



Analysis

Principal group:	–COOH	carboxylic acid
Parent hydride:		cyclohexane
Functionalized parent hydride		cyclohexanecarboxylic acid
Primary substituents:	–Cl	chloro
	–CH_2-CH_2-CH_2-CH_2-CH_2-CH_3	hexyl
Secondary substituents:	–Cl	chloro
	=O	oxo
	–CH_2-OH	hydroxymethyl
Substituted substituents:	4-chloro-2-(hydroxymethyl)-5-oxohexyl	

Together with other rules, this analysis leads to the preferred IUPAC name:
4,5-dichloro-2-[4-chloro-2-(hydroxymethyl)-5-oxohexyl]cyclohexane-1-carboxylic acid (PIN)

P-59.2.2 Seniority of heteroatoms over suffixes

Heterocyclic compounds and chains modified by skeletal replacement (‘a’) nomenclature are treated similarly. They are considered as parent compounds with a fixed numbering. As a consequence, heteroatoms have seniority for low locants and suffixes are assigned the next possible lowest locants.

Fixed numbering for heteroacyclic parent structures named by skeletal replacement (‘a’) nomenclature is a major change to Rule C-0.6 (ref. 1) in which principal characteristic groups and free valence were preferred over heteroatoms for low locants.

P-59.2.2.1 For chains the replacement operation is applied to the hydrocarbon parent hydride to create a new parent hydride with a fixed numbering. Suffixes receive the lowest possible locants in accordance with the resulting numbering.

Example:

$$\overset{1}{\mathrm{C}}\mathrm{H_3\text{-}CH_2\text{-}}\overset{3}{\mathrm{O}}\mathrm{\text{-}CH_2\text{-}CH_2\text{-}}\overset{6}{\mathrm{O}}\mathrm{\text{-}CH_2\text{-}CH_2\text{-}}\overset{9}{\mathrm{O}}\mathrm{\text{-}CH_2\text{-}CH_2\text{-}}\overset{12}{\mathrm{O}}\mathrm{\text{-}CH_2\text{-}CH_2\text{-}}\overset{15}{\mathrm{C}}\mathrm{OOH}$$

Analysis

Principal characteristic group:	–(C)OOH	oic acid
Hydrocarbon parent hydride:	CH_3-$[CH_2]_{13}$-CH_3	pentadecane
Skeletal replacement (‘a’) prefix	–O–	oxa

Heteroacyclic parent hydride:

$$\overset{1}{\mathrm{C}}\mathrm{H_3\text{-}CH_2\text{-}}\overset{3}{\mathrm{O}}\mathrm{\text{-}CH_2\text{-}CH_2\text{-}}\overset{6}{\mathrm{O}}\mathrm{\text{-}CH_2\text{-}CH_2\text{-}}\overset{9}{\mathrm{O}}\mathrm{\text{-}CH_2\text{-}CH_2\text{-}}\overset{12}{\mathrm{O}}\mathrm{\text{-}CH_2\text{-}CH_2\text{-}}\overset{15}{\mathrm{C}}\mathrm{H_3}$$

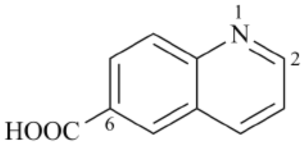
3,6,9,12-tetraoxapentadecane

Functionalized heteroacyclic parent hydride:

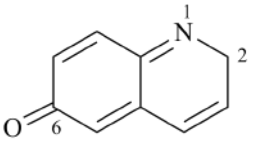
$$\overset{1}{\mathrm{C}}\mathrm{H_3\text{-}CH_2\text{-}}\overset{3}{\mathrm{O}}\mathrm{\text{-}CH_2\text{-}CH_2\text{-}}\overset{6}{\mathrm{O}}\mathrm{\text{-}CH_2\text{-}CH_2\text{-}}\overset{9}{\mathrm{O}}\mathrm{\text{-}CH_2\text{-}CH_2\text{-}}\overset{12}{\mathrm{O}}\mathrm{\text{-}CH_2\text{-}CH_2\text{-}}\overset{15}{\mathrm{C}}\mathrm{OOH}$$

Together with other rules, this analysis leads to the preferred IUPAC name:
3,6,9,12-tetraoxapentadecan-15-oic acid (PIN)

P-59.2.2.2 Heterocyclic compounds having retained or systematic names are considered as parent hydrides. Thus, suffixes are added and assigned lowest possible locants in accordance with the fixed numbering of the heterocyclic ring or ring system. Added indicated hydrogen atoms, if needed, are assigned next lowest possible locants.

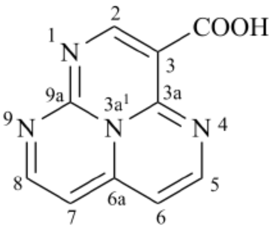


quinoline-6-carboxylic acid (PIN)



quinolin-6(2*H*)-one (PIN)

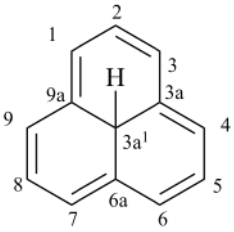
Example:



Analysis

Principal characteristic group: –COOH carboxylic acid

Hydrocarbon parent hydride:

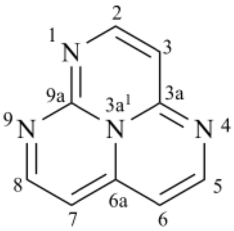


3a^1*H*-phenalene

[Note the new system of numbering for internal atoms in fused systems, 3a^1 in place of 9b; see P-25.3.3.3.]

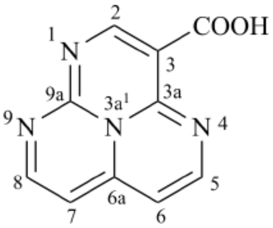
Skeletal replacement (‘a’) prefix –N< aza

Heterocyclic parent hydride:



1,3a^1,4,9-tetraazaphenalene

Functionalized heterocyclic parent hydride:

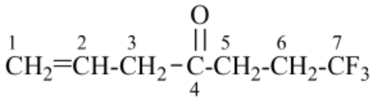


Together with other rules, this analysis leads to the preferred IUPAC name:
1,3a^1,4,9-tetraazaphenalene-3-carboxylic acid (PIN)

P-59.2.3 Seniority of suffixes over unsaturation

P-59.2.3.1 After suffixes, if there is a choice, low locants are assigned to ‘ene’ and ‘yne’ endings, and then to detachable prefixes, if applicable.

Example:



$$\overset{1}{CH_2}=\overset{2}{CH}-\overset{3}{CH_2}-\underset{4}{\overset{\overset{O}{||}}{C}}-\overset{5}{CH_2}-\overset{6}{CH_2}-\overset{7}{CF_3}$$

Analysis

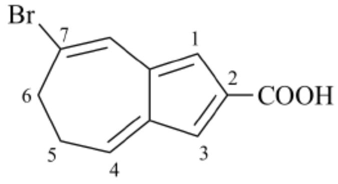
Principal characteristic group:	=O	one
Parent hydride:	$CH_3-[CH_2]_5-CH_3$	heptane
Functionalized parent hydride	$CH_3-[CH_2]_2-CO-[CH_2]_2-CH_3$	heptan-4-one
Substituent prefix	–F	fluoro

Together with other rules, this analysis leads to the preferred IUPAC name:
7,7,7-trifluorohept-1-en-4-one (PIN)

P-59.2.3.2 Hydro and dehydro prefixes are used to express a change in the degree of hydrogenation of the parent hydride. In these recommendations, these prefixes are considered detachable but only in the context of numbering; they are not included among the detachable substituent prefixes. In names, they are cited immediately before the name of the parent compound, after those of detachable substituent prefixes arranged in alphanumerical order.

In these recommendations, the prefixes ‘hydro’ and ‘dehydro’ are detachable, but are not included in the category of alphabetized detachable prefixes (see P-14.4; see also P-15.1.5.2, P-31.2, P-58.2), which is a change from recommendations in earlier editions (ref. 1, 2). When along with the endings 'ene' and 'yne' they are used to modify parent hydrides, they are regulated by the principle of lowest locants, in accord with the numbering of the parent hydride and after priority has been given to indicated hydrogen, 'added indicated hydrogen', and suffixes, when present, as specified in the general rules for numbering (P-14.4).

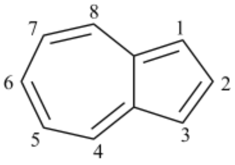
Example:



Analysis

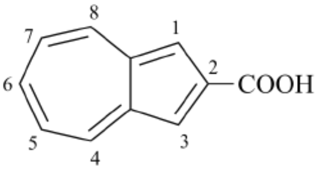
Principal characteristic group: –COOH carboxylic acid

Parent hydride:



azulene

Functionalized parent hydride



azulene-2-carboxylic acid

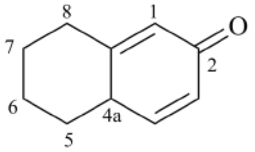
Saturation prefix –H dihydro

Substituent prefix –Br bromo

Together with other rules, this analysis leads to the preferred IUPAC name:
7-bromo-5,6-dihydroazulene-2-carboxylic acid (PIN)

P-59.2.3.3 Mancude ketones, imines, and other characteristic groups as well as free valences, such as '-ylidene' are named by the 'added indicated hydrogen' method. If there is a choice, indicated hydrogen atoms have priority for low locants, then suffixes, 'added indicated hydrogen' atoms, and finally hydro prefixes, in that order.

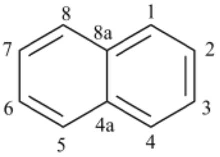
Example 1:



Analysis

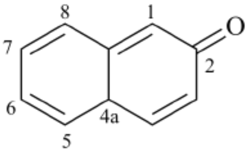
Principal characteristic group: =O one

Parent hydride:



naphthalene

Functionalized parent hydride

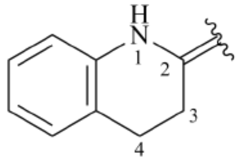


naphthalen-2(4a*H*)-one

Saturation prefix **4** –H tetrahydro

Together with other rules, this analysis leads to the preferred IUPAC name:
5,6,7,8-tetrahydronaphthalen-2(4a*H*)-one (PIN)

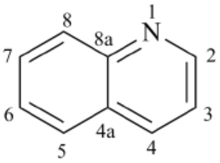
Example 2:



Analysis

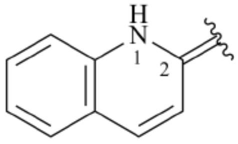
Free valences: R= ylidene

Parent hydride:



quinoline

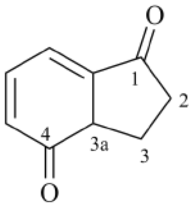
Parent hydride with
free valences



quinolin-2(1*H*)-ylidene

Together with other rules, this analysis leads to the preferred IUPAC name:
3,4-dihydroquinolin-2(1*H*)-ylidene (preferred prefix)

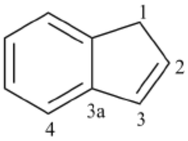
Example 3:



Analysis:

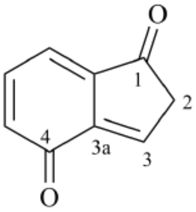
Principal characteristic group: =O dione

Parent hydride:



1*H*-indene

Functionalised parent hydride:

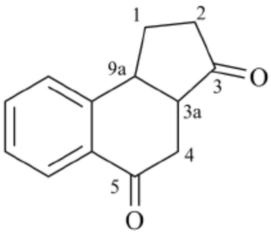


1*H*-indene-1,4(2*H*)-dione

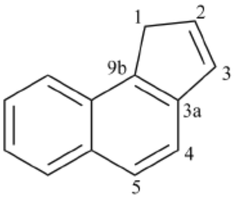
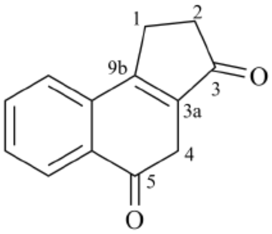
Saturation prefix: dihydro

Together with other rules, this analysis leads to the preferred IUPAC name:
3,3a-dihydro-1*H*-indene-1,4(2*H*)-dione

Example 4:



Analysis

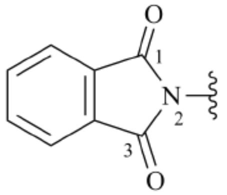
Principal characteristic group:	**2** =O	dione
Parent hydride:		1*H*-cyclopenta[*a*]naphthalene
Functionalized parent hydride		1*H*-cyclopenta[*a*]naphthalene-3,5(2*H*,4*H*)-dione

Explanation: See P-58.2.2

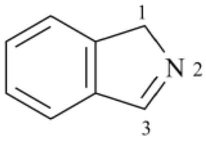
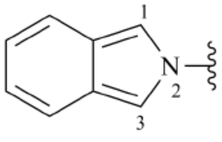
Saturation prefix	**2** –H	dihydro

Together with other rules, this analysis leads to the preferred IUPAC name:
3a,9b-dihydro-1*H*-cyclopenta[*a*]naphthalene-3,5(2*H*,4*H*)-dione (PIN)

Example 5:



Analysis

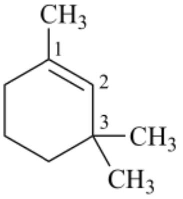
Principal characteristic group:	R–	yl
Parent hydride:		1*H*-isoindole
Parent hydride with free valence		2*H*-isoindol-2-yl
Saturation prefix	**2** –H	dihydro
Substituent:	=O	dioxo

Together with other rules, this analysis leads to the preferred IUPAC name:
1,3-dioxo-1,3-dihydro-2*H*-isoindol-2-yl (preferred prefix)

P-59.2.4 Seniority of 'ene' and 'yne' endings and hydro prefixes over detachable prefixes.

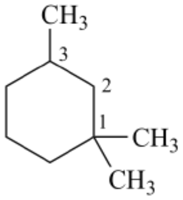
If there is a choice, low locants are assigned first to 'ene' and 'yne' endings and 'hydro/dehydro' prefixes, then to detachable alphabetized prefixes.

Examples:

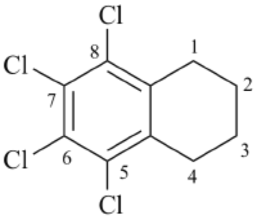


1,3,3-trimethylcyclohex-1-ene (PIN)

compare with

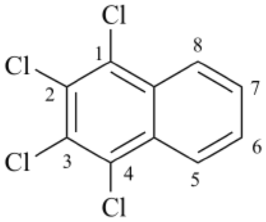


1,1,3-trimethylcyclohexane (PIN)



5,6,7,8-tetrachloro-1,2,3,4-hydronaphthalene (PIN)

compare with

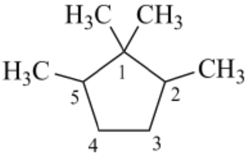


1,2,3,4-tetrachloronaphthalene (PIN)

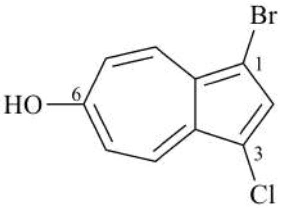
P-59.2.5 Treatment of detachable prefixes

If there is a choice, low locants are assigned to detachable prefixes considered together, and, if there is a further choice, in alphanumerical order.

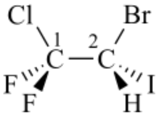
Examples:



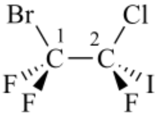
1,1,2,5-tetramethylcyclopentane (PIN)
(not 1,2,2,3-tetramethylcyclopentane;
the set of locants 1,1,2,5 is lower than 1,2,2,3.)



1-bromo-3-chloroazulen-6-ol (PIN)



(2*R*)-2-bromo-1-chloro-1,1-difluoro-2-iodoethane (PIN)



(2*S*)-1-bromo-2-chloro-1,1,2-trifluoro-2-iodoethane (PIN)

Chapter P-6 APPLICATIONS TO SPECIFIC CLASSES OF COMPOUNDS

(P-60 to P-65)
(continued with P-66 to P-69)

P-60 Introduction
P-61 Substitutive nomenclature: prefix mode
P-62 Amines and imines
P-63 Hydroxy compounds, ethers, peroxols, peroxides and chalcogen analogues
P-64 Ketones, pseudoketones and heterones, and chalcogen analogues
P-65 Acids, acyl halides and pseudohalides, salts, esters, and anhydrides
P-66 Amides, imides, hydrazides, nitriles, and aldehydes
P-67 Mononuclear and polynuclear noncarbon acids and their functional replacement analogues as functional parents for naming organic compounds
P-68 Nomenclature for organic compounds of the group 13, 14, 15, 16, and 17 elements not included in sections P-62 through P-67
P-69 Nomenclature for organometallic compounds

P-60 INTRODUCTION

The recommendations in this Chapter illustrate how the general principles and specific rules set out in the preceding sections are applied to various types of compounds.

P-60.1 TOPICAL OUTLINE

Section P-61 describes hydrocarbons that are named substitutively only by the prefix mode. It includes and exemplifies compounds formed by substituting parent hydrides by substituents derived from other parent hydrides and by characteristic groups that are always used as prefixes when applied to hydrocarbons.

Sections P-62 to P-66 include compounds that are named, in substitutive nomenclature, by suffixes and prefixes, and by means of other types of nomenclature. The traditional classes from acids to imines are described (see P-41).

Section P-67 describes nomenclature of organic derivatives of noncarbon acids and their functional replacement analogues.

Section P-68 covers the nomenclature of organic compounds of the Groups 13, 14, 15, 16, and 17 elements not included in Sections P-62 to P-67.

Section P-69 describes nomenclature for organometallic compounds.

P-60.2 PRESENTATION OF NAMES.

Names described in this Chapter are presented in a systematic way. General methods recommended to generate IUPAC preferred names are all described in a simplified way with reference to the following full descriptions:

(a) names formed substitutively using suffixes follow the general method described in P-15.1. Substitutive names are formed by adding a suffix such as ‘al’ ‘ol’, ‘yl’, ‘carbaldehyde’, ‘carboxylic acid’, etc., to the name of a parent hydride, with elision of the final letter ‘e’ of the parent hydride, if any, before ‘a’, ‘i’, ‘o’, ‘u’, and ‘y’;

(b) names formed substitutively by using prefixes follow the general method. Substitutive names are formed by adding a prefix such as amino, hydroxy, etc., to the name of the parent hydride or parent compound; in order to preserve their formal identity, there is no elision of the last letter of these prefixes;

(c) names formed by functional class nomenclature follow the general method described in P-15.2. Functional class names are formed by citing the name of the class, such as alcohol, oxide, ketone, etc., preceded by the name of the substituent groups cited in alphabetical order and separated by a space, if required;

(d) names formed by skeletal replacement (‘a’) nomenclature follow the methodology described in P-15.4;

(e) functional parents are discussed in terms of preferred names and names that can be used in general nomenclature.

The method to generate preferred IUPAC names is indicated by a phrase such as 'This method generates preferred IUPAC names' or 'Method (1) leads to preferred IUPAC names'. The abbreviation 'PIN' is placed after names that are 'preferred IUPAC names'. Names that were recommended in the past but are not included in these recommendations are described parenthetically by the phrase 'no longer recommended'. For example, the prefix 'methylene' is 'no longer recommended' in IUPAC nomenclature to designate the $=CH_2$ group.

Names preceded by 'not' are names that are not constructed in accordance with the rule as described in this Chapter. Thus, they are 'incorrect names'. As they are not alternatives to preferred IUPAC names, they must not be used. For example, the name 'ethanolamine', which is still widely used, is badly constructed because of the presence of two suffixes; it is not an alternative to the preferred IUPAC name, '2-aminoethan-1-ol'.

P-61 SUBSTITUTIVE NOMENCLATURE: PREFIX MODE

P-61.0 Introduction
P-61.1 General methodology
P-61.2 Hydrocarbyl groups and corresponding di- and polyvalent groups
P-61.3 Halogen compounds
P-61.4 Diazo compounds
P-61.5 Nitro and nitroso compounds
P-61.6 Heterones
P-61.7 Azides
P-61.8 Isocyanates
P-61.9 Isocyanides
P-61.10 Fulminates and isofulminates
P-61.11 Polyfunctional compounds

P-61.0 INTRODUCTION

This subsection describes the names of compounds formed by substitutive nomenclature that includes only prefixes denoting substituent groups and/or characteristic groups. These prefixes are detachable and cited in a name in alphanumerical order.

Hydrocarbyl groups and their corresponding polyvalent groups (substituent groups derived from hydrocarbon parent hydrides) are included in this subsection because they occupy the penultimate rank in the seniority order of classes (see P-41) and thus are treated as prefixes in presence of a higher class. A similar situation prevails for halogen compounds in their standard bonding number, which are at the bottom in the order of seniority of classes (see P-41).

Diazo compounds, nitro and nitroso compounds, azides, isocyanates, isocyanides, and fulminates/isofulminates are also included in this Section. Ethers, peroxides, and acetals are not considered in this Section, but are treated at length in association with hydroxy compounds and aldehydes (see P-63.2, P-63.3, and P-66.6.5, respectively).

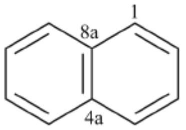
The characteristic groups described here (see Table 5.1) are referred to as 'characteristic groups denoted, in substitutive nomenclature, only as prefixes' (see R-4.1, ref. 2). This statement must not be interpreted as a must for always using these characteristic groups as prefixes. Substitutive nomenclature is based on a seniority system based on classes. The senior class must be determined first (see P-41).

P-61.1 GENERAL METHODOLOGY

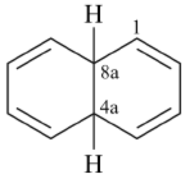
Substitutive nomenclature is based on the substitutive operation involving the exchange of one or more hydrogen atoms of a parent hydride or parent compound for another atom or group. This process is expressed by either a prefix or suffix denoting the atom or group being introduced. Substitution is not possible when no hydrogen atoms are present. However, if hydrogen atoms are added to a structure by an additive operation (to a double bond, for example), substitution then becomes possible. The formal addition of hydrogen atoms must precede the substitution operation when atoms or groups denoted by prefixes are involved; thus, they are cited after the alphabetized prefixes.

> This is a change from previous recommendations. In these recommendations the prefix 'hydro' is detachable but not alphabetized with other substituent prefixes. In names, it is cited immediately before the name of the parent hydride, after alphabetized prefixes and before nondetachable prefixes.

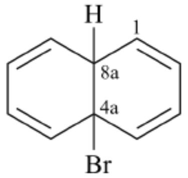
Examples:



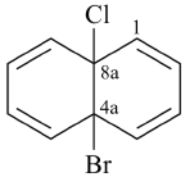
naphthalene (PIN)



4a,8a-dihydronaphthalene (PIN)



4a-bromo-4a,8a-dihydronaphthalene (PIN)



4a-bromo-8a-chloro-4a,8a-dihydronaphthalene (PIN)

The seniority order of parent structures, the principal chain, and the senior ring system are chosen in accordance with Rule P-44.

When there is a choice for numbering, the general rule described in P-14.4 is applied. The starting point and the direction of numbering of a compound are chosen so as to give lowest locants to the following structural features (if present) considered successively in the order given until a decision is reached:

(a) fixed numbering, as for naphthalene, bicyclo[2.2.2]octane, etc.;

(b) heteroatoms in heterocycles and in acyclic parent structures;

This is a change for acyclic parent structures. Heteroatoms in chains are now considered as part of the parent hydride and, as such, have seniority over suffixes for numbering.

(c) indicated hydrogen [for unsubstituted compounds; a higher locant may be needed at another position to provide for a substituent suffix in accordance with structural feature (d)];

(d) principal group named as suffix;

(e) added indicated hydrogen (consistent with the structure of the compound and in accordance with further substitution);

(f) saturation/unsaturation (‘hydro’/‘dehydro’ prefixes) or unsaturation (‘ene’/‘yne’ endings);

In acyclic parent structures the order of seniority between unsaturation and length of chain given in earlier recommendations is reversed. Thus, the first criterion to be considered in choosing a preferred parent acyclic chain is the length of the chain; unsaturation is now the second criterion.

(g) substituents named as prefixes (low locants are allocated for substituents regardless of kind; then, if necessary, in the order of citation in the name).

P-61.2 HYDROCARBYL GROUPS AND CORRESPONDING DI- AND POLYVALENT GROUPS

Only substituted hydrocarbons are discussed here. For substitution on other parent hydrides see P-68.1 for Group 13, P-68.2 for Group 14, P-68.3 for Group 15, P-68.4 for Group 16, and P-68.5 for Group 17.

Substituted hydrocarbons for which a parent hydride name is not available (see Chapter P-2) have a name that consists of a parent hydride name and appropriate substitutive prefixes derived from other parent hydrides.

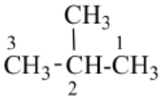
P-61.2.1 Acyclic hydrocarbons

Names of substituted acyclic hydrocarbons are formed substitutively by selecting the principal chain in accordance with rule P-44. This rule has been modified from previous rules; seniority is now given to the length of the chain rather than to unsaturation (see P-44.3).

In a change from previous recomendations, the order of seniority between unsaturation and length of chain given in earlier recommendations is reversed. Thus, the first criterion to be considered in choosing a preferred parent acyclic chain is the length of the chain; unsaturation is now the second criterion.

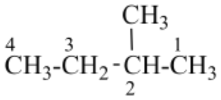
The name ‘isoprene’ is retained, but no substitution is allowed. (see P-31.1.2.1). The names ‘isobutane’, ‘isopentane’ and ‘neopentane’ are no longer recommended.

Examples:



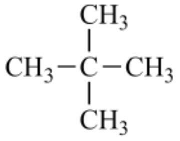
$$\overset{3}{C}H_3-\underset{2}{\overset{\overset{\displaystyle CH_3}{|}}{C}}H-\overset{1}{C}H_3$$

2-methylpropane (PIN)
(not isobutane)



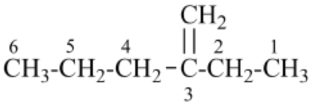
$$\overset{4}{C}H_3-\overset{3}{C}H_2-\underset{2}{\overset{\overset{\displaystyle CH_3}{|}}{C}}H-\overset{1}{C}H_3$$

2-methylbutane (PIN)
(not isopentane)



$$CH_3-\underset{\underset{\displaystyle CH_3}{|}}{\overset{\overset{\displaystyle CH_3}{|}}{C}}-CH_3$$

2,2-dimethylpropane (PIN)
(not neopentane)



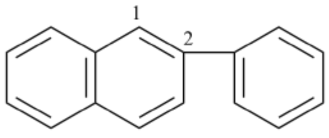
$$\overset{6}{C}H_3-\overset{5}{C}H_2-\overset{4}{C}H_2-\underset{3}{\overset{\overset{\displaystyle CH_2}{||}}{C}}-\overset{2}{C}H_2-\overset{1}{C}H_3$$

3-methylidenehexane (PIN)
(not 2-ethylpent-1-ene; the longer chain now supersedes
a shorter unsaturated chain; see P-44.3)

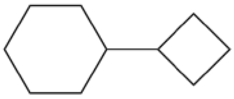
P-61.2.2 Cyclic hydrocarbons

Names of rings or cyclic systems substituted by rings or ring systems are formed in accordance with the seniority order of rings and ring systems (see P-44.2.1 and P-44.4.1).

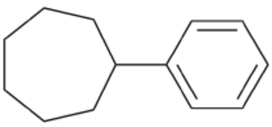
Examples:



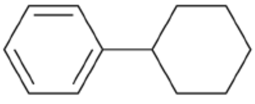
2-phenylnaphthalene (PIN)
(naphthalene, having two rings, is senior to benzene, that has only one ring; see P-44.2.1)



cyclobutylcyclohexane (PIN)
(cyclohexane has more ring atoms than cyclobutane; see P-44.2.1)



phenylcycloheptane (PIN)
(cycloheptane has more ring atoms than benzene; see P-44.2.1)



cyclohexylbenzene (PIN)
(benzene has more multiple bonds than cyclohexane; see P-44.4.1)

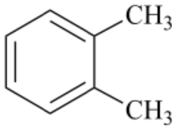
P-61.2.3 Hydrocarbons consisting of rings and chains.

Names of cyclic hydrocarbons substituted by chains are formed by substituting chains, saturated or unsaturated, into rings (see P-44.1.2.2). This rule must be strictly applied in the context of preferred IUPAC names. The name 'toluene' is retained with no substitution allowed for preferred IUPAC names, but substitution is allowed on both the ring and side chain with certain restrictions (see P-22.1.3) for general nomenclature. The name 'xylene' is a preferred IUPAC name, but cannot be substituted and the name 'mesitylene' can only be used in general nomenclature and cannot be substituted.

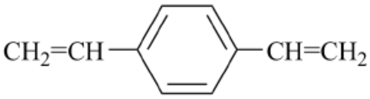
The names 'styrene', 'stilbene' and 'fulvene' are retained only for general nomenclature. Styrene and stilbene can be ring substituted as prescribed in P-31.1.3.4. There is no substitution allowed for 'fulvene' (see P-31.1.3.4).

In the 1993 Guide (ref. 2), these parent hydrides were retained but only limited substitution was allowed.

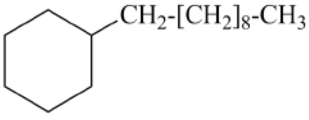
Examples:



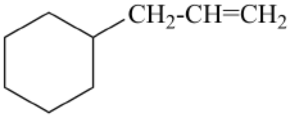
1,2-xylene (PIN)
1,2-dimethylbenzene
(not *o*-methyltoluene,
substitution of toluene by additional methyl groups is not allowed: see P-22.1.3)



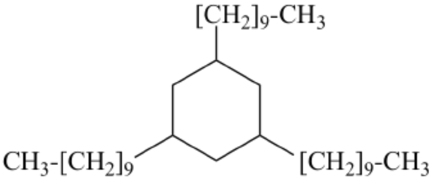
1,4-diethenylbenzene (PIN)
1,4-divinylbenzene



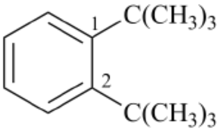
decylcyclohexane (PIN)
(ring preferred to chain, see P-52.2.8)
1-cyclohexyldecane



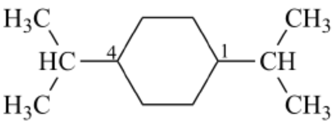
(prop-2-en-1-yl)cyclohexane (PIN)
(ring preferred to chain, see P-52.2.8)
3-cyclohexylprop-1-ene
allylcyclohexane



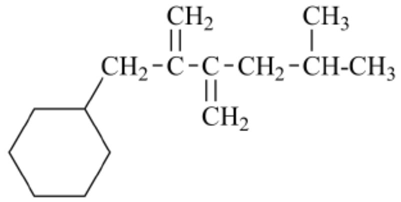
1,3,5-tri(decyl)cyclohexane (PIN)
(not 1,3,5-tris(decyl)cyclohexane)



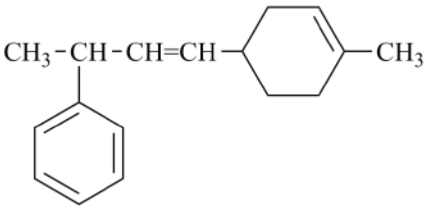
1,2-di-*tert*-butylbenzene (PIN)



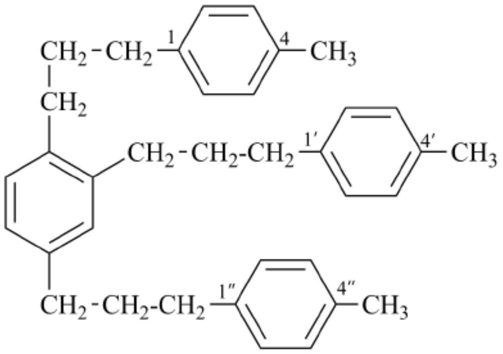
1,4-di(propan-2-yl)cyclohexane (PIN)


CH2
CH3
CH2-C-C-CH2-CH-CH3
CH2

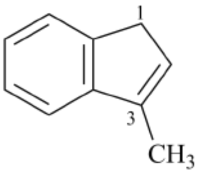
(5-methyl-2,3-dimethylidenehexyl)cyclohexane (PIN)
[not [2-methylidene-3-(2-methylpropyl)but-3-en-1-yl]cyclohexane;
the longer chain is preferred to the shorter unsaturated chains, see P-44.3]


CH3-CH-CH=CH
CH3

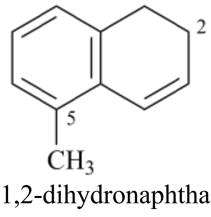
[4-(4-methylcyclohex-3-en-1-yl)but-3-en-2-yl]benzene [PIN; see P-44.3]
{not [1-methyl-3-(4-methylcyclohex-3-en-1-yl)prop-2-en-1-yl]benzene;
the longest chain is preferred to the shorter chains}


CH2-CH2
1
4
CH3
CH2
CH2-CH2-CH2
1′
4′
CH3
CH2-CH2-CH2
1″
4″
CH3

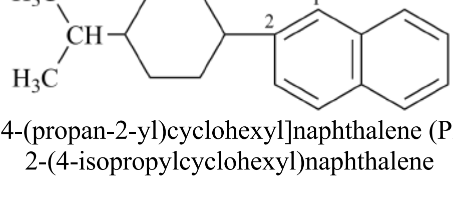
1,1′,1″-[benzene-1,2,4-triyltri(propane-3,1-diyl)]tris(4-methylbenzene) (PIN)
(multiplicative name, numbering shown, see P-51.3)
1,2,4-tris[3-(4-methylphenyl)propyl]benzene



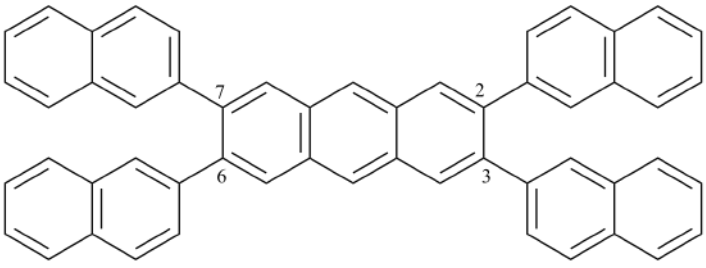
3-methyl-1*H*-indene (PIN)



5-methyl-1,2-dihydronaphthalene (PIN)


H3C
CH
H3C
2
1

2-[4-(propan-2-yl)cyclohexyl]naphthalene (PIN)
2-(4-isopropylcyclohexyl)naphthalene

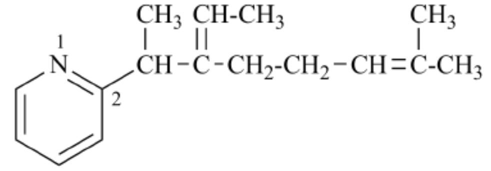


2,3,6,7-tetra(naphthalen-2-yl)anthracene (PIN)

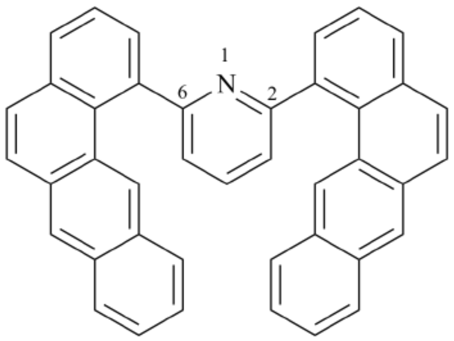
P-61.2.4 Structures containing heterocycles

Names of heterocyclic rings or ring systems substituted by chains or rings or ring systems are formed in accordance with the seniority order of rings or ring systems over chains (see P-44.1.2.2) and with the seniority order of rings and ring systems (see P-44.2).

Examples:



2-(3-ethylidene-7-methyloct-6-en-2-yl)pyridine (PIN)
(preferred parent substituent prefix, see P-46.1)
2-(2-ethylidene-1,6-dimethylhept-5-en-1-yl)pyridine



2,6-bis(benzo[*a*]anthracen-1-yl)pyridine
2,6-di(tetraphen-1-yl)pyridine (PIN)

P-61.3 HALOGEN COMPOUNDS

Halogen compounds in which the halogen atom is in its standard bonding number are always expressed by prefixes in substitutive nomenclature or, as the principal characteristic group or in functional class nomenclature as a separate word.

P-61.3.1 Halogen compounds in which the halogen atom is in its standard bonding number are named in two ways:

(1) by substitutive nomenclature, using the prefixes ‘bromo’, ‘chloro’, ‘fluoro’, and ‘iodo’ and appropriate multiplicative prefixes, as required;

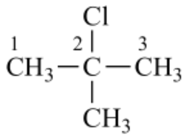
(2) by functional class nomenclature, in which names are formed by citing the name of the organic ‘groups’ followed by the class name ‘fluoride’, ‘chloride’, ‘bromide’, or ‘iodide’, as a separate word, preceded, if necessary, by a multiplicative prefix. Functional class names usually are used to denote simple structures, having one kind of halogen, and are not used to name more complex structures. Additive names, such as stilbene dibromide, are not recommended.

Method (1) leads to preferred IUPAC names (see P-51.1).

Examples:

CH_3-I
iodomethane (PIN)
methyl iodide

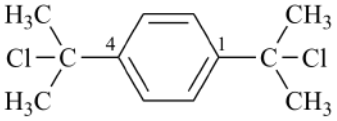
C_6H_5-CH_2-Br
(bromomethyl)benzene (PIN;
no substitution on toluene)
α-bromotoluene
(for toluene substitution rules in general nomenclature; see P-22.1.3)
benzyl bromide



$$\begin{array}{c}\mathrm{Cl}\\ | \\ \overset{1}{\mathrm{CH_3}}-\overset{2}{\mathrm{C}}-\overset{3}{\mathrm{CH_3}}\\ | \\ \mathrm{CH_3}\end{array}$$

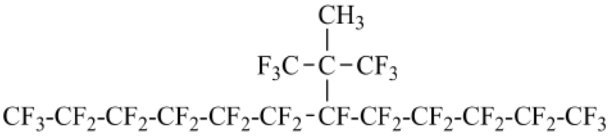
2-chloro-2-methylpropane (PIN)
tert-butyl chloride

$\mathrm{Br\text{-}}\overset{1}{\mathrm{C}}\mathrm{H_2\text{-}}\overset{2}{\mathrm{C}}\mathrm{H_2\text{-}Br}$
1,2-dibromoethane (PIN)
ethylene dibromide



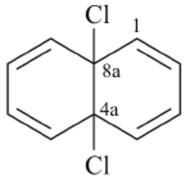
1,4-bis(2-chloropropan-2-yl)benzene (PIN)
1,4-bis(1-chloro-1-methylethyl)benzene

$\mathrm{C_6H_5\text{-}}\overset{1}{\mathrm{C}}\mathrm{HBr\text{-}}\overset{2}{\mathrm{C}}\mathrm{HBr\text{-}C_6H_5}$
1,1′-(1,2-dibromoethane-1,2-diyl)dibenzene (PIN;
multiplicative name, see P-51.3)
1,2-dibromo-1,2-diphenylethane (substitutive name)
(not stilbene dibromide)

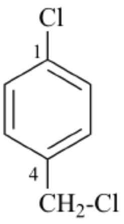


$$\begin{array}{c}\mathrm{CH_3}\\ | \\ \mathrm{F_3C-C-CF_3}\\ | \\ \mathrm{CF_3\text{-}CF_2\text{-}CF_2\text{-}CF_2\text{-}CF_2\text{-}CF_2\text{-}CF\text{-}CF_2\text{-}CF_2\text{-}CF_2\text{-}CF_2\text{-}CF_3}\end{array}$$

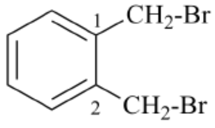
1,1,1,2,2,3,3,4,4,5,5,6,6,7,8,8,9,9,10,10,11,11,12,12,12-pentacosafluoro-7-(1,1,1,3,3,3-hexafluoro-2-methylpropan-2-yl)dodecane (PIN)
1,1,1,2,2,3,3,4,4,5,5,6,6,7,8,8,9,9,10,10,11,11,12,12,12-pentacosafluoro-7-[2,2,2-trifluoro-1-methyl-1-(trifluoromethyl)ethyl]dodecane



4a,8a-dichloro-4a,8a-dihydronaphthalene (PIN)



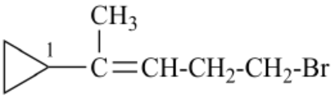
1-chloro-4-(chloromethyl)benzene (PIN)
α,4-dichlorotoluene
(for substitution rules for toluene in general nomenclature; see P-22.1.3)



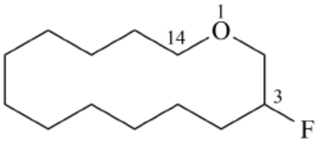
1,2-bis(bromomethyl)benzene (PIN)
α-bromo-2-(bromomethyl)toluene
(for rules on substitution rules of toluene in general nomenclature, see P-22.1.3
[not α,α′-dibromo-*o*-xylene (no substitution on xylene, see P-22.1.3]

$\overset{6}{\mathrm{C}}\mathrm{H_3\text{-}}\overset{5}{\mathrm{C}}\mathrm{H_2\text{-}}\overset{4}{\mathrm{C}}\mathrm{H_2\text{-}}\overset{3}{\mathrm{C}}\mathrm{H_2\text{-}}\overset{2}{\mathrm{C}}\mathrm{HCl\text{-}}\overset{1}{\mathrm{C}}\mathrm{H_3}$
2-chlorohexane (PIN)
hexan-2-yl chloride
1-methylpentyl chloride

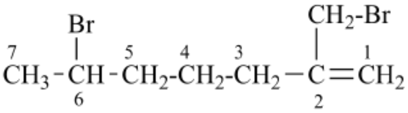
$F_2N\text{-}CO\text{-}NF_2$
tetrafluorourea (PIN)
tetrafluorocarbonic diamide



(5-bromopent-2-en-2-yl)cyclopropane (PIN)
(ring preferred to chain, see P-44.1.2.2;
preferred substituent prefix, see P-46.1)
(4-bromo-1-methylbut-1-en-1-yl)cyclopropane
5-bromo-2-cyclopropylpent-2-ene

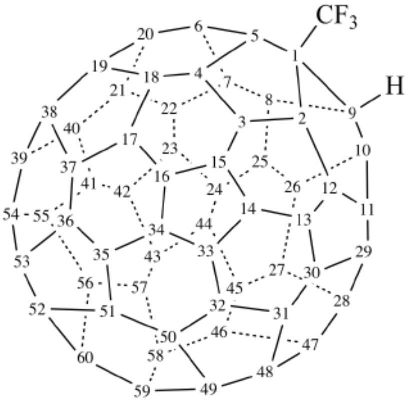


3-fluoro-1-oxacyclotetradecane (PIN)
1-oxacyclotetradecan-3-yl fluoride

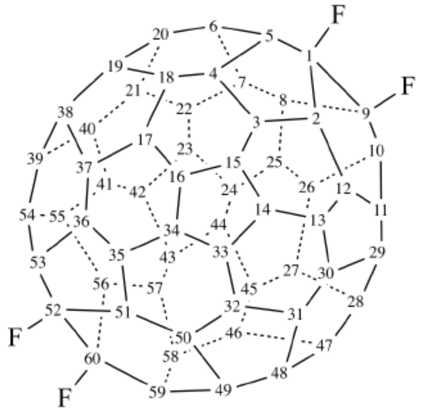


$\overset{7}{C}H_3\text{-}\underset{6}{\overset{Br}{\overset{|}{C}}}H\text{-}\overset{5}{C}H_2\text{-}\overset{4}{C}H_2\text{-}\overset{3}{C}H_2-\underset{2}{\overset{CH_2\text{-}Br}{\overset{|}{C}}}=\overset{1}{C}H_2$

6-bromo-2-(bromomethyl)hept-1-ene (PIN)
2-methylideneheptane-1,6-diyl dibromide



1-(trifluoromethyl)-1,9-dihydro(C_{60}-I_h)[5,6]fullerene (PIN)



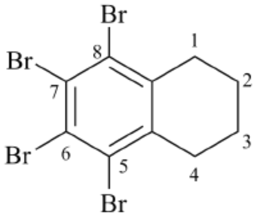
1,9,52,60-tetrafluoro-1,9,52,60-tetrahydro(C_{60}-I_h)[5,6]fullerene (PIN)
(C_{60}-I_h)[5,6]fullerene-1,9,52,60-tetrayl tetrafluoride

$\overset{1}{C}H_3\text{-}\overset{2}{Si}H_2\text{-}CH_2\text{-}\overset{4}{Si}H_2\text{-}CH_2\text{-}\overset{6}{Si}H_2\text{-}CH_2\text{-}\overset{8}{Si}H_2\text{-}CH_2\text{-}\overset{10}{C}H_2\text{-}Cl$
10-chloro-2,4,6,8-tetrasiladecane (PIN)
2,4,6,8-tetrasiladecan-10-yl chloride

$\overset{1}{C}H_2\text{=}CH\text{-}CH_2\text{-}CH_2\text{-}\overset{5}{C}H_2\text{-}I$
5-iodopent-1-ene (PIN)
pent-4-en-1-yl iodide

$\mathrm{Br\text{-}\overset{1}{C}H_2\text{-}CH_2\text{-}\overset{3}{C}H{=}CH\text{-}CH_2\text{-}\overset{6}{C}H_3}$

1-bromohex-3-ene (PIN)
hex-3-en-1-yl bromide



5,6,7,8-tetrabromo-1,2,3,4-tetrahydronaphthalene (PIN)
5,6,7,8-tetrahydronaphthalene-1,2,3,4-tetrayl tetrabromide
(for position of ‘hydro’/‘dehydro’ prefixes in preferred IUPAC names, see P-31.2.1)

P-61.3.2 Halogen atoms attached to heteroatoms

P-61.3.2.1 In P-61.3.1, halogen atoms in their standard bonding number are attached to carbon atoms. The halogen atoms can also be attached to heteroatoms. The prefixes ‘bromo’, ‘chloro’, ‘fluoro’, and ‘iodo’ are used to name halogen compounds when the halogen atoms are attached to B, Al, In, Ga, Tl, Si, Ge, Sn, Pb, and Bi.

Examples:

$\mathrm{Cl\text{-}B(CH_3)_2}$
chlorodi(methyl)borane (PIN;
borane is a preselected name; see P-12.2)
dimethylboranyl chloride

$\mathrm{Cl_3Si\text{-}CH_2I}$
trichloro(iodomethyl)silane (PIN;
silane is a preselected name; see P-12.2)

$\mathrm{F_2Ge{=}CH_2}$
difluoro(methylidene)germane (PIN;
germane is a preselected name; see P-12.2)

$\mathrm{H_2P\text{-}PH\text{-}Cl}$
chlorodiphosphane (preselected name;
diphosphane is a preselected name see P-12.2)

P-61.3.2.2 In naming any compound, its class and its seniority must be determined in accordance with the seniority of classes described in P-41. Halogen atoms linked to nitrogen atoms generate amides of inorganic acids that are senior to halo compounds described in P-61.3.1. Similarly, acid halides or esters of inorganic acids may be created when the halogen atoms are linked to phosphorus or chalcogen atoms. Names must be based on the seniority of classes; some names that were recommended in past recommendations may still be used in general nomenclature.

Examples:

$\mathrm{CH_3\text{-}NH\text{-}Cl}$
methylhypochlorous amide (PIN; see P-68.5.3)
N-chloromethanamine

$\mathrm{CH_3\text{-}PH\text{-}Cl}$
methylphosphinous chloride (PIN; see P-67.1.2.5)
chloro(methyl)phosphane

$\mathrm{CH_3\text{-}S\text{-}Cl}$
methyl thiohypochlorite (PIN; see P-67.1.3)

P-61.3.2.3 Compounds containing the groups –XO, $\mathrm{–XO_2}$, or $\mathrm{–XO_3}$ (X = halogen) are expressed by the following compulsory prefixes in substitutive nomenclature:

–XO chlorosyl (no longer chloroso), bromosyl, iodosyl, fluorosyl

$\mathrm{–XO_2}$ chloryl (no longer chloroxy), bromyl, iodyl, fluoryl

$\mathrm{–XO_3}$ perchloryl, perbromyl, periodyl, perfluoryl

Examples:

$\mathrm{C_6H_5\text{-}ClO_3}$
perchlorylbenzene (PIN)

C_6H_5-IO
iodosylbenzene (PIN)

P-61.3.3 Compounds containing the group –I(OH)$_2$ or similar groups are named substitutively by using prefixes based on the preselected parent hydride name λ^3-iodane (see P-21.1 2.1 and P-68.5.1)

P-61.3.4 Retained names

The retained names ‘bromoform’ for $HCBr_3$, ‘chloroform’ for $HCCl_3$, and ‘iodoform’ for HCI_3 are acceptable in general nomenclature. Preferred IUPAC names are substitutive names.

Example:

$HCBr_3$
bromoform
tribromomethane (PIN)

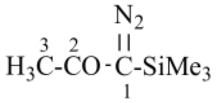
P-61.4 DIAZO COMPOUNDS

Compounds containing a group =N_2 attached to a single carbon atom are named by adding the prefix ‘diazo’ to the name of the parent hydride or functional parent hydride (see also P-74.2.2.2.3).

Examples:

CH_2N_2
diazomethane (PIN)

N_2CH-CO-O-C_2H_5
ethyl diazoacetate (PIN)



$$H_3\overset{3}{C}\text{-}\overset{2}{C}O\text{-}\underset{1}{\overset{N_2}{\overset{||}{C}}}\text{-}SiMe_3$$

1-diazo-1-(trimethylsilyl)propan-2-one (PIN)
1-diazo-1-(trimethylsilyl)acetone

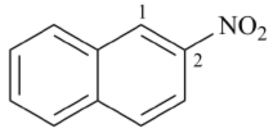
P-61.5 NITRO AND NITROSO COMPOUNDS

P-61.5.1 Nitro and nitroso compounds

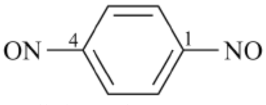
Compounds containing the –NO_2 or –NO group are named by means of the prefixes ‘nitro’ and ‘nitroso’, respectively, unless these groups can be named on the basis of the parent structures nitric and nitrous acids, NO_2-OH and NO-OH, respectively, or their corresponding esters, anhydrides, amides and hydrazides. Derivatives of nitric acid and nitrous acids are described in Section P-67. Acid halides and pseudohalides are described in P-67.1.2.5; amides and hydrazides in P-67.1.2.6; salts, esters and anhydrides in P-67.1.3.

Examples:

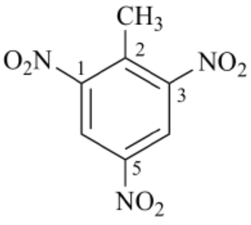
CH_3-NO_2
nitromethane (PIN)



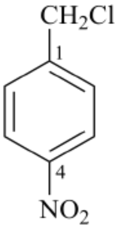
2-nitronaphthalene (PIN)



1,4-dinitrosobenzene (PIN)



2-methyl-1,3,5-trinitrobenzene (PIN)
2,4,6-trinitrotoluene (for substitution rules for toluene
in general nomenclature, see P-22.1.3



1-(chloromethyl)-4-nitrobenzene (PIN)
α-chloro-4-nitrotoluene (for substitution rules for toluene
in general nomenclature, see P-22.1.3
4-nitrobenzyl chloride

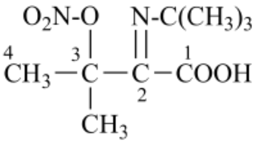
$CH_3\text{-}BH\text{-}NO_2$
methyl(nitro)borane (PIN)

$(CH_3)_3Si\text{-}NO_2$
trimethyl(nitro)silane (PIN)

$CH_3\text{-}\overset{1}{P}H\text{-}\overset{2}{P}H\text{-}NO$
1-methyl-2-nitrosodiphosphane (PIN)

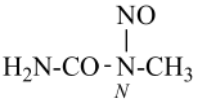
P-61.5.2 In the presence of a characteristic group having seniority to be named as a suffix or a parent structure, nitro and nitroso groups can be attached to any atom. When linked to another nitrogen atom they are not considered to lengthen the nitrogen chain.

Examples:



$$\overset{4}{C}H_3{-}\overset{O_2N\text{-}O}{\underset{CH_3}{\overset{3}{C}}}{-}\overset{N\text{-}C(CH_3)_3}{\underset{2}{\overset{\|}{C}}}{-}\overset{1}{C}OOH$$

2-(*tert*-butylimino)-3-methyl-3-(nitrooxy)butanoic acid (PIN)



$$H_2N\text{-}CO\text{-}\overset{NO}{\underset{N}{N}}\text{-}CH_3$$

N-methyl-*N*-nitrosourea (PIN)

P-61.5.3 *aci*-Nitro compounds

Compounds containing the group =N(O)OH are named as derivatives of azinic acid, $H_2N(O)\text{-}OH$, a preselected name, and by using the prefix name hydroxy(oxo)-λ^5-azanylidene, when a characteristic group having priority for citation as a suffix is present. The use of the prefix '*aci*-nitro' may be used in general nomenclature (see P-67.1.6).

Example:

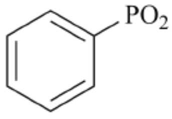
$CH_3\text{-}CH{=}N(O)\text{-}OH$
ethylideneazinic acid (PIN)
aci-nitroethane

P-61.6 HETERONES

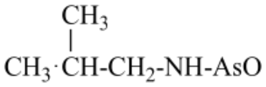
Compounds containing the –PO, –PO_2, –AsO or –AsO_2 are called heterones (see P-64.1.2.2, P-64.4). In the presence of a more senior characteristic group they are described by the compound prefixes oxophosphanyl, dioxo-λ^5-phosphanyl, oxoarsanyl, and dioxo-λ^5-arsanyl.

Note: In spite of the use of the term 'phospho' to describe the –PO_2 group as a substituent prefix since 1937, the term 'phospho' is widely used in biochemical nomenclature in place of phosphono for designating the –$P(O)(OH)_2$ group linked to a heteroatom, as in phosphocholine and 6-phospho-D-glucose; and as an infix to describe phosphoric diesters, as in glycerophosphocholine. Consequently, in these recommendations the term 'phospho', and collaterally the terms phosphoroso, arso, and arsenoso, which are still used in CAS index nomenclature, are no longer used.

Examples:



phenyl-λ^5-phosphanedione (PIN)
dioxo(phenyl)-λ^5-phosphane
(not phosphobenzene)



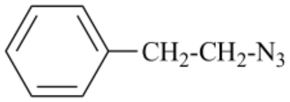
$CH_3{\cdot}\overset{\overset{\displaystyle CH_3}{|}}{C}H\text{-}CH_2\text{-}NH\text{-}AsO$

[(2-methylpropyl)amino]arsanone (PIN)
N-(2-methylpropyl)-1-oxoarsanamine
(not *N*-arsenoso-2-methylpropanamine)

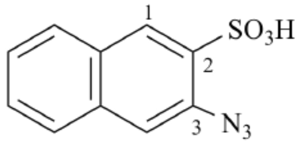
P-61.7 AZIDES

Compounds containing a $–N_3$ ($–N{=}N^+{=}N^–$) group attached to a parent hydride, are named using substitutive nomenclature and the prefix ‘azido’. This method gives preferred IUPAC names rather than names based on the class name ‘azido’ in functional class nomenclature (see also P-74.2.2.2.2).

Examples:



(2-azidoethyl)benzene (PIN)
2-phenylethyl azide
(not phenethyl azide)



3-azidonaphthalene-2-sulfonic acid (PIN)

P-61.8 ISOCYANATES

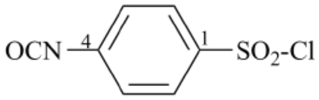
> This is a change from previous recommendations. Preferred IUPAC names are generated substitutively using the prefix ‘isocyanato’ attached directly to a parent hydride. Previously, functional class names were recommended for this class.

Compounds containing the –N=C=O group attached to a parent hydride structure, are named by using substitutive nomenclature and the prefix ‘isocyanato’. This method leads to preferred IUPAC names rather than names based on functional class nomenclature and the functional class name ‘isocyanate’. Chalcogen analogues are named by inserting the functional replacement infix ‘thio’, ‘seleno’, or ‘telluro’ into the names ‘isocyanate’ or ‘isocyanato’ just after ‘iso’.

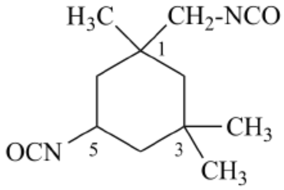
Examples:

C_6H_{11}-NCO
isocyanatocyclohexane (PIN)
cyclohexyl isocyanate

C_6H_5-NCS
isothiocyanatobenzene (PIN)
phenyl isothiocyanate



4-isocyanatobenzene-1-sulfonyl chloride (PIN)



5-isocyanato-1-(isocyanatomethyl)-1,3,3-trimethylcyclohexane (PIN)
3-(isocyanatomethyl)-3,5,5-trimethylcyclohexyl isocyanate

H_3Si-NCS
isothiocyanatosilane (PIN;
silane is a preselected name; see P-12.2)

H_2B-NCO
isocyanatoborane(PIN;
borane is a preselected name; see P-12.2)

Note: In accordance with the seniority order of classes, the isocyanato group and its chalcogen analogues form acid pseudohalides when attached to the central atom P, As, Sb of inorganic acids (see P-67.1.2.5); these acid pseudohalides have priority over the isocyanates and their chalcogen analogues formed by substitution. See also pseudoketones P-64.3.

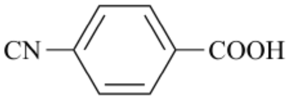
P-61.9 ISOCYANIDES

This is a change in these recommendations. Preferred IUPAC names are formed substitutively using the prefix 'isocyano' attached directly to a parent hydride. Previously, functional class names were recommended for this class.

Compounds containing the –NC group attached to a parent hydride structure, are named by substitutive nomenclature and the prefix 'isocyano'. This method leads to preferred IUPAC names rather than names based on functional class nomenclature and the functional class name 'isocyanide'.

Examples:

C_6H_5-NC
isocyanobenzene (PIN)
phenyl isocyanide



4-isocyanobenzoic acid (PIN)

P-61.10 FULMINATES AND ISOFULMINATES

The structure of fulminic acid was indicated in the 1979 Recommendations (Rule C-833.1, ref. 1) and in the 1993 Recommendations (Rule R-5.7.9.2, ref. 2) as HO-N≡C, and its derivatives were denoted by the class name fulminate and the prefix fulminato. Although consistent with the pseudohalogen cyanate, the structure of this acid in the literature is claimed to be HCNO. Accordingly, the name fulminic acid and that of its substituent group fulminato are not acceptable nor are the names isofulminic acid and isofulminate. The IUPAC preferred name for the structure HCNO is formonitrile oxide (see P-66.5.4.1) and the IUPAC preferred name for its isomer, HO-N=C**:**, is based on hydroxylamine (see P-68.3.1.1.1).

This is a change from the potentially ambiguous names fulminate and fulminato in previous recommendations to systematic substitutive names.

Examples:

H-C≡N=O
formonitrile oxide (PIN)

–C≡N=O
(oxo-λ^5-azanylidyne)methyl (preferred prefix)
(not isofulminato)

HO-N=C
λ^2-methylidenehydroxylamine
N-hydroxy-λ^2-methanamine (PIN)

–O-N=C
(λ^2-methylideneamino)oxy (preferred prefix)
(not fulminato)

P-61.11 POLYFUNCTIONAL COMPOUNDS

In substitutive names, detachable prefixes (except for 'hydro'/'dehydro' prefixes), are cited in alphanumerical order. Low locants are assigned to:

This is a change from previous recommendations. In these recommendations the prefixes 'hydro' and 'dehydro' are detachable but not alphabetized with other substituent prefixes. In names, they are cited immediately before the name of the parent hydride, after alphabetized prefixes and before nondetachable prefixes.

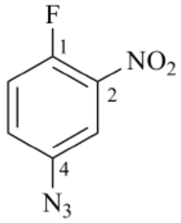
(1) the prefixes as a set, and if there is a choice,

(2) to the prefix that is cited first in a name.

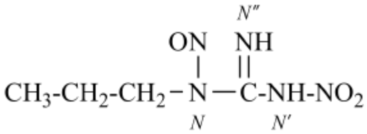
In functional class nomenclature, names are formed following the order for compound classes (see P-41) and the order of seniority for halides and pseudohalides (see P-41 and P-65.5.2.1) to choose the principal characteristic group. Names formed substitutively rather than functional class names are preferred IUPAC names.

P-61.11.1 Low locants are assigned as a set, without regard to kind.

Examples:



4-azido-1-fluoro-2-nitrobenzene (PIN)
4-azido-2-nitrophenyl fluoride



$$\mathrm{CH_3\text{-}CH_2\text{-}CH_2-}\underset{N}{\overset{\mathrm{ON}}{\overset{|}{\mathrm{N}}}}-\underset{N'}{\overset{\overset{N''}{\mathrm{NH}}}{\overset{\|}{\mathrm{C}}}}\mathrm{\text{-}NH\text{-}NO_2}$$

N′-nitro-*N*-nitroso-*N*-propylguanidine (PIN)

P-61.11.2 Low locants are assigned to the prefix cited first in the name

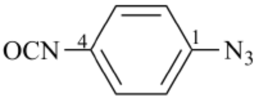
Examples:

$$\overset{1}{\mathrm{Cl_3Si}}\text{-}\overset{2}{\mathrm{SiH_2}}\text{-}\overset{3}{\mathrm{SiH_2}}\text{-}\overset{4}{\mathrm{SiH_2}}\text{-}\overset{5}{\mathrm{Si}}\mathrm{(CH_3)_3}$$

1,1,1-trichloro-5,5,5-trimethylpentasilane (PIN)
(pentasilane is a preselected name, see P-12.2)

$$\mathrm{Br\text{-}}\overset{1}{\mathrm{CH_2}}\text{-}\overset{2}{\mathrm{CH_2}}\mathrm{\text{-}Cl}$$

1-bromo-2-chloroethane (PIN)



1-azido-4-isocyanatobenzene (PIN)
4-isocyanatophenyl azide

P-62 AMINES AND IMINES

P-62.0 Introduction
P-62.1 General methodology
P-62.2 Amines
P-62.3 Imines
P-62.4 *N*-Substitution of amines and imines by heteroatoms
P-62.5 Amine oxides, imine oxides and chalcogen analogues
P-62.6 Amine and imine salts

P-62.0 INTRODUCTION

The nomenclature of amines and imines is rich in traditions and a variety of methods have been used for constructing their names (see refs. 1 and 2). The rationalization necessary to define preferred IUPAC names is the appropriate opportunity to establish proper names for amines and imines and retain clear and unambiguous methods for choosing the appropriate parent and naming individual compounds.

Rules C-11.4 and C-811-C-815 in the 1979 Recommendations (ref. 1) are superseded, as well as Rules R-5.4.1–R-5.4.3 in the 1993 Recommendations (ref. 2).

P-62.1 GENERAL METHODOLOGY

The general methodology is based on the following principles:

(a) definitions, as given in the Glossary of Class Names Based on Structure (ref. 23), classify amines and imines unambiguously as follows;

(1) monoamines are compounds formally derived from ammonia (NH_3) by replacing one, two, or three of its hydrogen atoms by one, two, or three hydrocarbyl groups by single bonds, thus having the general structures R-NH_2 (primary amines), R_2NH (secondary amines), R_3N (tertiary amines);

(2) imines are compounds having the structure $R_2C{=}NR$ (R = H or hydrocarbyl), corresponding either to ketimines, $RR'C{=}NR''$ or to aldimines, $RCH{=}NR'$;

(b) amines are senior to imines in the seniority order of classes;

(c) methods for naming amines and imines will be restricted to a minimum, preference being given to the substitutive method using the suffixes 'amine' and 'imine';

(d) a minimum of traditional names will be retained;

(e) polyamines are further classified as follows;

(1) simple polyamines are compounds in which all amino groups are attached to the same parent hydride;

(2) complex polyamines are compounds in which a choice between two or more parent hydrides must be made.

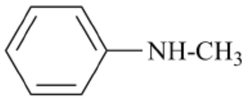
P-62.2 AMINES

P-62.2.1 Primary amines

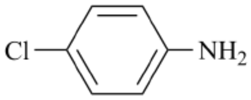
P-62.2.1.1 Retained names

P-62.2.1.1.1 Aniline, for C_6H_5-NH_2 , is the only name for a primary amine retained as a preferred IUPAC name for which full substitution is permitted on the ring and the nitrogen atom. It is a Type 2a retained name; for the rules of substitution see P-15.1.8.2. Substitution is limited to substituent groups cited as prefixes in accordance with the seniority of functional groups explicitly expressed or implied in the functional parent compound name. The name benzenamine may be used in general nomenclature. The prefix name 'anilino' is retained as the preferred prefix for C_6H_5-NH– with full substitution allowed. The name 'phenylamino' may be used in general nomenclature.

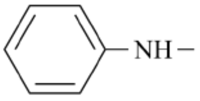
Examples:



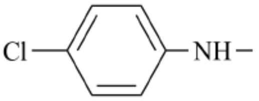
N-methylaniline (PIN)
N-methylbenzenamine



4-chloroaniline (PIN)
4-chlorobenzenamine



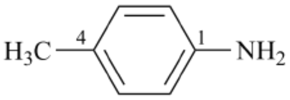
anilino (preferred prefix)
phenylamino



4-chloroanilino (preferred prefix)
(4-chlorophenyl)amino

P-62.2.1.1.2 The names 'toluidine', 'anisidine', and 'phenetidine' for which *o*-, *m*-, and *p*- have been used to distinguish isomers, and 'xylidine' for which numerical locants, such as 2,3-, have been used, are no longer recommended, nor are the corresponding prefixes 'toluidino', 'anisidino', 'phenetidino', and 'xylidino'.

Examples:



4-methylaniline (PIN)
4-methylbenzenamine
(not *p*-toluidine)

4-methylanilino (preferred prefix)
(4-methylphenyl)amino
(not *p*-toluidino)

P-62.2.1.2 Primary amines, R-NH$_2$, are systematically named in the following ways:

(1) by adding the suffix ‘amine’ to the name of the parent hydride;

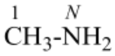
(2) by adding the name of the substituent group R– to the parent hydride ‘azane’;

(3) by adding the name of the substituent group R– to the term ‘amine’ used as a preselected parent hydride name for NH$_3$; this method is used only with monoamines.

Note: Amine is not a true preselected parent hydride. In these recommendations, it is considered as a ‘pseudo’ parent hydride, based on the premise that this method originated by modification of a functional class name based on the class name amine, for example, ethyl amine. The space in the functional class name is eliminated to form the current name ethylamine

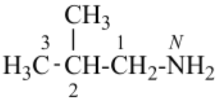
Method (1) leads to preferred IUPAC names.

Examples:



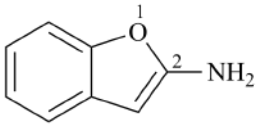
$\overset{1}{\mathrm{CH_3}}\text{-}\overset{N}{\mathrm{NH_2}}$

(1) methanamine (PIN)
(2) methylazane
(3) methylamine

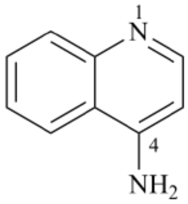


$\mathrm{H_3C}\text{-}\underset{2}{\overset{\overset{\mathrm{CH_3}}{3\,|}}{\mathrm{CH}}}\text{-}\overset{1}{\mathrm{CH_2}}\text{-}\overset{N}{\mathrm{NH_2}}$

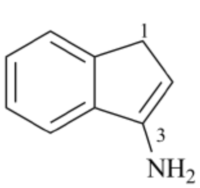
(1) 2-methylpropan-1-amine (PIN)
(2) (2-methylpropyl)azane
(3) (2-methylpropyl)amine



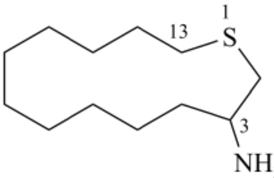
1-benzofuran-2-amine (PIN)
(1-benzofuran-2-yl)azane
(1-benzofuran-2-yl)amine



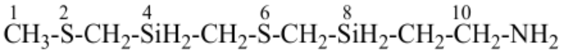
quinolin-4-amine (PIN)
(quinolin-4-yl)azane
(quinolin-4-yl)amine
4-quinolylamine



1*H*-inden-3-amine (PIN)
(1*H*-inden-3-yl)azane
(1*H*-inden-3-yl)amine

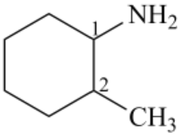


1-thiacyclotridecan-3-amine (PIN)
(1-thiacyclotridecan-3-yl)azane
(1-thiacyclotridecan-3-yl)amine

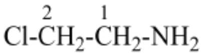


$\overset{1}{C}H_3\text{-}\overset{2}{S}\text{-}CH_2\text{-}\overset{4}{Si}H_2\text{-}CH_2\text{-}\overset{6}{S}\text{-}CH_2\text{-}\overset{8}{Si}H_2\text{-}CH_2\text{-}\overset{10}{C}H_2\text{-}NH_2$

2,6-dithia-4,8-disiladecan-10-amine (PIN)
(2,6-dithia-4,8-disiladecan-10-yl)azane
(2,6-dithia-4,8-disiladecan-10-yl)amine



2-methylcyclohexan-1-amine (PIN)
(2-methylcyclohexyl)azane
(2-methylcyclohexyl)amine



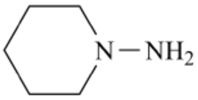
$Cl\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}H_2\text{-}NH_2$

2-chloroethan-1-amine (PIN)
(2-chloroethyl)azane
(2-chloroethyl)amine

P-62.2.1.3 Amino groups, i.e., $–NH_2$, attached to heteroatoms

When attached to heteroatoms, amino groups are expressed as suffixes when representing the principal characteristic group.

Examples:



piperidin-1-amine (PIN)
(piperidin-1-yl)azane
(piperidin-1-yl)amine

$(CH_3)_3Si\text{-}NH_2$
1,1,1-trimethylsilanamine (PIN)
(trimethylsilyl)azane
(trimethylsilyl)amine

P-62.2.2 Secondary and tertiary amines

P-62.2.2.1 Symmetrical and unsymmetrical secondary and tertiary amines are named only by the same methods described in P-62.2.1.2.

(1) substitutively using the retained name ‘aniline’ or the suffix ‘amine’ and the name of a parent hydride with further *N*-substitution;

(2) substitutively, by prefixing, in alphabetical order when required, the name(s) of the substituent group(s) R, R′ or R″ to the parent hydride name ‘azane’. In order to avoid ambiguity, the second prefix in a secondary amine, and the second and the third prefixes in a tertiary amines must be enclosed in parentheses when these prefixes denote simple substituents.

(3) substitutively, by prefixing, in alphabetical order when required, the name(s) of the substituent group(s) R, R′ or R″ to the parent hydride name ‘amine’. In order to avoid ambiguity, the second prefix in a secondary amine, and the second and the third prefixes in a tertiary amines must be enclosed in parentheses when these prefixes denote simple substituents.

Method (1) generates preferred IUPAC names. Functional parent names like diethylamine and triethylamine are deprecated. The prefixes in names of such secondary and tertiary amines formed by method (3) are set off by parentheses to distinguish them from these deprecated names.

Examples:

$C_6H_5\text{-}\overset{N}{N}H\text{-}C_6H_5$

(1) *N*-phenylaniline (PIN)
(2) diphenylazane
(3) (diphenyl)amine
(not azanediyldibenzene;
the retained name ‘aniline’ must be used for all its *N* derivatives)

$(CH_3\text{-}CH_2)_2\overset{N}{N}\text{-}\overset{1}{C}H_2\text{-}\overset{2}{C}H_3$

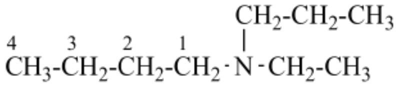
(1) *N*,*N*-diethylethanamine (PIN)
(2) triethylazane
(3) (triethyl)amine

$Cl\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}H_2\text{-}\overset{N}{N}H\text{-}CH_2\text{-}CH_2\text{-}Cl$

2-chloro-*N*-(2-chloroethyl)ethan-1-amine (PIN)
bis(2-chloroethyl)azane
bis(2-chloroethyl)amine
(not 2,2′-dichlorodiethylamine)

$\overset{3}{C}H_3\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}H_2\text{-}\overset{N}{N}H\text{-}CH_2\text{-}CH_2\text{-}Cl$

(1) *N*-(2-chloroethyl)propan-1-amine (PIN)
(2) (2-chloroethyl)(propyl)azane
(3) (2-chloroethyl)(propyl)amine
[not *N*-(2-chloroethyl)propylamine]

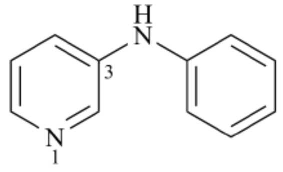


$\overset{4}{C}H_3\text{-}\overset{3}{C}H_2\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}H_2\text{-}\overset{\overset{\textstyle CH_2\text{-}CH_2\text{-}CH_3}{|}}{N}\text{-}CH_2\text{-}CH_3$

(1) *N*-ethyl-*N*-propylbutan-l-amine (PIN)
(2) butyl(ethyl)(propyl)azane
(3) butyl(ethyl)(propyl)amine
(not *N*-ethyl-*N*-propylbutylamine)

$H_3Si\text{-}NH\text{-}SiH_3$

(1) *N*-silylsilanamine (preselected name)
(2) disilylazane
(3) (disilyl)amine
(not disilazane; see P-21.2.3.1)

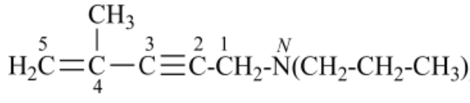


(1) *N*-phenylpyridin-3-amine (PIN)
(2) phenyl(pyridin-3-yl)azane
(3) phenyl(pyridin-3-yl)amine
[not *N*-(pyridin-3-yl)aniline]

P-62.2.2.2 Selection of the principal chain or senior ring system in secondary and tertiary amines.

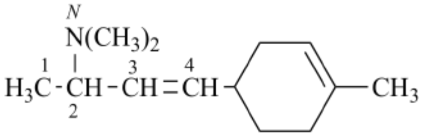
Names of amines formed substitutively by using the retained name aniline or the suffix ‘amine’ are based on a principal chain and a senior ring system (see P-44.1). When a choice for parent hydride is possible between a ring and a chain, the ring is preferred. In names using ‘amine’ as a parent hydride, substituent groups expressed as prefixes are cited in alphanumerical order; the prefix(es) immediately preceding the term ‘amine’ is (are) enclosed in parentheses.

Examples:

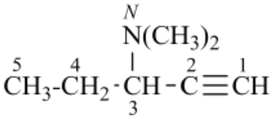


$H_2\overset{5}{C}{=}\underset{4}{\overset{\overset{\textstyle CH_3}{|}}{C}}{-}\overset{3}{C}{\equiv}\overset{2}{C}\text{-}\overset{1}{C}H_2\text{-}\overset{N}{N}(CH_2\text{-}CH_2\text{-}CH_3)_2$

(1) 4-methyl-*N*,*N*-dipropylpent-4-en-2-yn-1-amine (PIN)
(2) (4-methylpent-4-en-2-yn-1-yl)di(propyl)azane
(3) (4-methylpent-4-en-2-yn-1-yl)di(propyl)amine



N,*N*-dimethyl-4-(4-methylcyclohex-3-en-1-yl)but-3-en-2-amine (PIN)
dimethyl[4-(4-methylcyclohex-3-en-1-yl)but-3-en-2-yl]azane
dimethyl[4-(4-methylcyclohex-3-en-1-yl)but-3-en-2-yl]amine

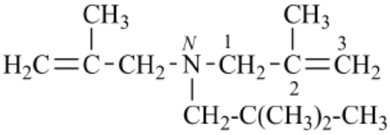


$\overset{5}{C}H_3\text{-}\overset{4}{C}H_2\text{-}\underset{3}{\overset{\overset{N}{N}(CH_3)_2}{CH}}\text{-}\overset{2}{C}\equiv\overset{1}{C}H$

N,*N*-dimethylpent-1-yn-3-amine (PIN)
dimethyl(pent-1-yn-3-yl)azane
dimethyl(pent-1-yn-3-yl)amine

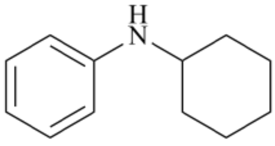
$\overset{4}{C}H_3\text{-}\overset{3}{C}H_2\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}H_2\text{-}\overset{N}{N}H\text{-}CH{=}CH_2$

N-ethenylbutan-1-amine (PIN)
butyl(ethenyl)azane
butyl(ethenyl)amine

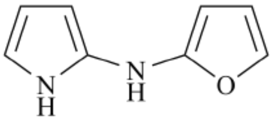


$H_2C{=}\overset{CH_3}{C}\text{-}CH_2\text{-}\underset{CH_2\text{-}C(CH_3)_2\text{-}CH_3}{\overset{N}{N}}\text{-}\overset{1}{C}H_2\text{-}\underset{2}{\overset{CH_3}{C}}{=}\overset{3}{C}H_2$

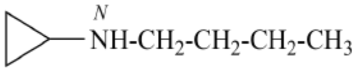
N-(2,2-dimethylpropyl)-2-methyl-*N*-(2-methylprop-2-en-1-yl)prop-2-en-1-amine (PIN)
(2,2-dimethylpropyl)bis(2-methylprop-2-en-1-yl)azane
(2,2-dimethylpropyl)bis(2-methylprop-2-en-1-yl)amine



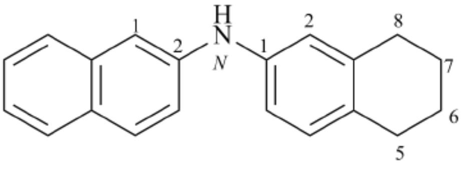
N-cyclohexylaniline (PIN)
cyclohexyl(phenyl)azane
cyclohexyl(phenyl)amine



N-(furan-2-yl)-1*H*-pyrrol-2-amine (PIN)
(furan-2-yl)(1*H*-pyrrol-2-yl)azane
2-furyl(1*H*-pyrrol-2-yl)azane
(furan-2-yl)(1*H*-pyrrol-2-yl)amine
2-furyl(1*H*-pyrrol-2-yl)amine



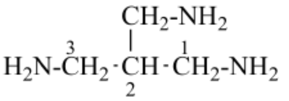
N-butylcyclopropanamine (PIN)
butyl(cyclopropyl)azane
(not *N*-cyclopropylbutan-1-amine)
butyl(cyclopropyl)amine



N-(5,6,7,8-tetrahydronaphthalen-2-yl)naphthalen-2-amine (PIN)
2-naphthyl(5,6,7,8-tetrahydro-2-naphthyl)azane
2-naphthyl(5,6,7,8-tetrahydro-2-naphthyl)amine
[not 5,6,7,8-tetrahydrodi(2-naphthyl)amine]

P-62.2.3 When all amino groups cannot be expressed as suffixes, or when the $–NH_2$ group is not the principal characteristic group, the prefix ‘amino’ is used in preferred IUPAC names. The prefix azanyl may be used in general nomenclature. The substituent prefix name ‘anilino’ is a preferred IUPAC prefix and substitution is allowed (see P-62.2.1.1.1).

Examples:

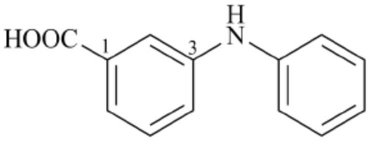


$$\underset{\overset{3}{}}{H_2N\text{-}\overset{3}{C}H_2\text{-}\underset{2}{\overset{\overset{CH_2\text{-}NH_2}{|}}{C}H}\text{-}\overset{1}{C}H_2\text{-}NH_2}$$

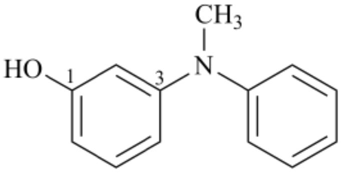
2-(aminomethyl)propane-1,3-diamine (PIN)
2-(azanylmethyl)propane-1,3-diamine

$H_2N\text{-}\overset{3}{C}H_2\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}OOH$

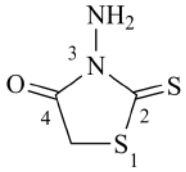
3-aminopropanoic acid (PIN)
3-azanylpropanoic acid



3-anilinobenzoic acid (PIN)
3-(phenylamino)benzoic acid



3-(*N*-methylanilino)phenol (PIN)
3-[methyl(phenyl)amino]phenol



3-amino-2-sulfanylidene-1,3-thiazolidin-4-one (PIN)
3-amino-2-thioxo-1,3-thiazolidin-4-one
(see also P-64.6.1)

Preferred IUPAC names for prefixes corresponding to –NHR, –NRR′, or $–NR_2$ are formed by prefixing the names of the groups R and R′ to the prefix ‘amino’, for example ‘methylamino’ for $–NH\text{-}CH_3$. Prefixes such as azanyl and azanylidene may be used in general nomenclature.

Examples:

$(CH_3NH)_2\overset{4}{C}H\text{-}\overset{3}{C}H_2\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}OOH$

4,4-bis(methylamino)butanoic acid (PIN)
4,4-bis(methylazanyl)butanoic acid

$(H_3Si)_2N\text{-}CH_2\text{-}COOH$
N,*N*-disilylglycine
(disilylamino)acetic acid
(disilylazanyl)acetic acid
[not (disilazan-2-yl)acetic acid]

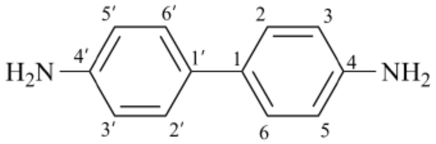
$H_3Si\text{-}HN\text{-}SiH_2–$
(silylamino)silyl (preselected prefix)
(silylazanyl)silyl
(not disilazan-1-yl)

P-62.2.4 Polyamines

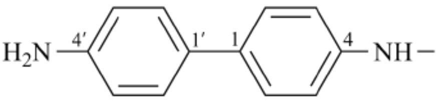
P-62.2.4.1 Simple polyamines are compounds in which all amino groups are attached to the same parent hydride

P-62.2.4.1.1 There are no retained names for simple polyamines that are used as preferred IUPAC names. However, in general nomenclature the name ‘benzidine’ may be used but only for the 4,4′-isomer, with substitution allowed as described in P-15.1.8.2 for a Type 2 retained name. The prefix ‘benzidino’ is retained with full substitution.

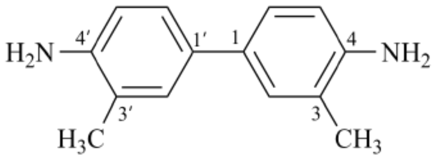
Examples:



benzidine
[1,1′-biphenyl]-4,4′-diamine (PIN)



benzidino
(4′-amino[1,1′-biphenyl]-4-yl)amino (preferred prefix)



3,3′-dimethylbenzidine
3,3′-dimethyl[1,1′-biphenyl]-4,4′-diamine (PIN)

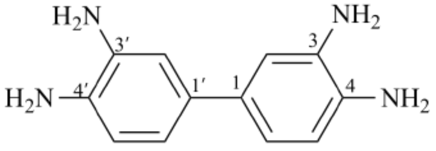
Di- and triamines, etc. are named similarly to monoamines. The locant of the parent hydride to which the nitrogen atom is attached is cited as a superscript to the letter locant *N*, for example, N^2, N^5, etc..

P-62.2.4.1.2 Two or more 'amine' groups attached to the same parent hydride are indicated by an appropriate multiplying numerical prefix 'di', 'tri', 'tetra', etc. The terminal letter 'a' of a numerical prefix is elided before the suffix amine, i. e., 'tetramine', not 'tetraamine'. Numerical locants, including '1' in the case of amines derived from mononuclear parent hydrides, are used to denote substitution on atoms of the parent hydride and '*N*' locants for substitution on the nitrogen atom for amines named by method (1). Method (2) is used only for monoamines.

Examples:

$H_2\overset{N^2}{N}\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}H_2\text{-}\overset{N^1}{N}H_2$

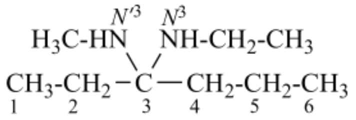
ethane-1,2-diamine (PIN)
ethylenediamine



[1,1′-biphenyl]-3,3′,4,4′-tetramine (PIN;
note the elision of 'a' from 'tetra' in 'tetramine')

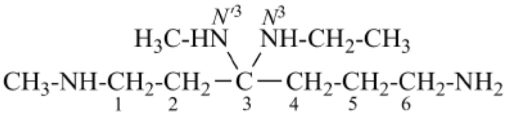
$CH_3\text{-}\overset{N^3}{N}H\text{-}\overset{3}{C}H_2\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}H_2\text{-}\overset{N^1}{N}H\text{-}CH_2\text{-}CH_3$

N^1-ethyl-N^3-methylpropane-1,3-diamine (PIN)



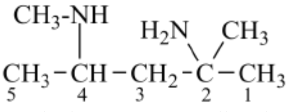
$$\underset{1}{C}H_3\text{-}\underset{2}{C}H_2-\underset{3}{\overset{H_3C\text{-}H\overset{N'^3}{N}\ \ \overset{N^3}{N}H\text{-}CH_2\text{-}CH_3}{C}}-\underset{4}{C}H_2\text{-}\underset{5}{C}H_2\text{-}\underset{6}{C}H_3$$

N^3-ethyl-N'^3-methylhexane-3,3-diamine (PIN)



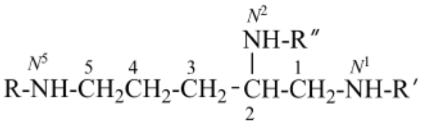
$$CH_3\text{-}NH\text{-}\underset{1}{C}H_2\text{-}\underset{2}{C}H_2-\underset{3}{\overset{H_3C\text{-}H\overset{N'^3}{N}\ \ \overset{N^3}{N}H\text{-}CH_2\text{-}CH_3}{C}}-\underset{4}{C}H_2\text{-}\underset{5}{C}H_2\text{-}\underset{6}{C}H_2\text{-}NH_2$$

N^3-ethyl-N^1,N'^3-dimethylhexane-1,3,3,6-tetramine (PIN)



$$\underset{5}{C}H_3-\underset{4}{\overset{CH_3\text{-}NH}{C}}H-\underset{3}{C}H_2\text{-}\underset{2}{\overset{H_2N\ \ CH_3}{C}}-\underset{1}{C}H_3$$

N^4,2-dimethylpentane-2,4-diamine (PIN)



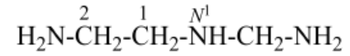
$R\text{-}NH\text{-}CH_2CH_2\text{-}CH_2\text{-}CH(NH\text{-}R'')\text{-}CH_2\text{-}NH\text{-}R'$

R = R′ = R″ = H pentane-1,2,5-triamine (PIN)
R = R′ = H; R″ = $-CH_3$ *N*²-methylpentane-1,2,5-triamine (PIN)
R = H; R′ = $-CH_3$; R″ = $-CH_2\text{-}CH_3$ *N*²-ethyl-*N*¹-methylpentane-1,2,5-triamine(PIN)

P-62.2.4.1.3 Complex polyamines, i.e., compounds in which a choice between two or more parent hydrides must be made, are systems composed of two or more secondary and/or tertiary amines.

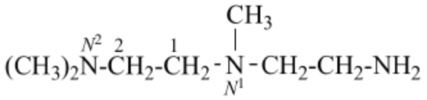
In complex polyamines a senior parent amine structure must be chosen. The senior parent amine structure is chosen in accordance with the choice of a principal chain or a senior ring or ring system, as described in P-44, or the preferred IUPAC name must be chosen in accordance with P-45. Alphanumerical order is applied when necessary. Multiplicative nomenclature, skeletal replacement ('a') nomenclature, or phane nomenclature are used when the conditions required by these types of nomenclature are fulfilled.

Examples:



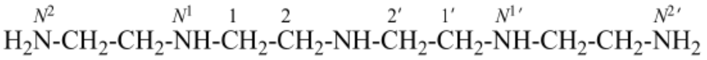
$H_2N\text{-}CH_2\text{-}CH_2\text{-}NH\text{-}CH_2\text{-}NH_2$

*N*¹-(aminomethyl)ethane-1,2-diamine (PIN)
[regular substitutive nomenclature;
the diamine having the longest carbon chain is chosen as parent structure; see P-44.3]



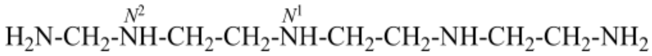
$(CH_3)_2N\text{-}CH_2\text{-}CH_2\text{-}N(CH_3)\text{-}CH_2\text{-}CH_2\text{-}NH_2$

*N*¹-(2-aminoethyl)-*N*¹,*N*²,*N*²-trimethylethane-1,2-diamine (PIN; numbering shown)
(the most substituted diamine is chosen as parent structure; P-45.2.1)
[not *N*¹,*N*¹-dimethyl-2,2′-(methylazanediyl)di(ethan-1-amine);
even in general nomenclature the parent name must be a diamine;
ethanamine is a monoamine]



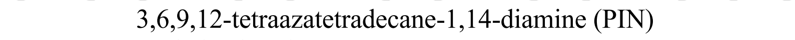
$H_2N\text{-}CH_2\text{-}CH_2\text{-}NH\text{-}CH_2\text{-}CH_2\text{-}NH\text{-}CH_2\text{-}CH_2\text{-}NH\text{-}CH_2\text{-}CH_2\text{-}NH_2$

*N*¹,*N*¹′-[azanediyldi(ethane-2,1-diyl)]di(ethane-1,2-diamine) [PIN;
the parent structure is a diamine and multiplicative nomenclature (see P-15.3; P-51.3; P-62.2.5)
allows four amine characteristic groups to be included in the name; numbering shown]
*N*¹-(2-aminoethyl)-*N*²-{2-[(2-aminoethyl)amino]ethyl}ethane-1,2-diamine (substitutive name)
[not 2,2′-azanediylbis[*N*-(2-aminoethyl)ethan-1-amine] [substitutive name;
even in general nomenclature, the parent structure must be a diamine; ethanamine is a monoamine]



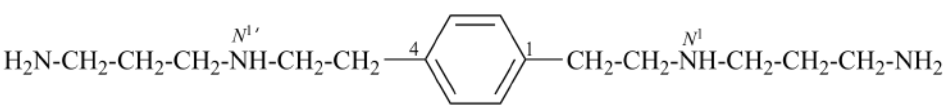
$H_2N\text{-}CH_2\text{-}NH\text{-}CH_2\text{-}CH_2\text{-}NH\text{-}CH_2\text{-}CH_2\text{-}NH\text{-}CH_2\text{-}CH_2\text{-}NH_2$

*N*¹-{2-[(2-aminoethyl)amino]ethyl}-*N*²-(aminomethyl)ethane-1,2-diamine (PIN)
[not *N*²-(aminomethyl)-*N*¹-{2-[(2-aminoethyl)amino]ethyl}ethane-1,2-diamine;
'aminoethyl' precedes 'aminomethyl' in alphanumerical order; P-14.5]
[not *N*¹-(2-aminoethyl)-*N*²-(aminomethyl)-2,2′-azanediyldi(ethan-1-amine);
the preferred IUPAC name must be a diamine]

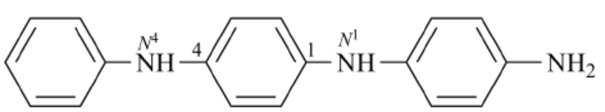


$H_2N\text{-}CH_2\text{-}CH_2\text{-}NH\text{-}CH_2\text{-}CH_2\text{-}NH\text{-}CH_2\text{-}CH_2\text{-}NH\text{-}CH_2\text{-}CH_2\text{-}NH\text{-}CH_2\text{-}CH_2\text{-}NH_2$

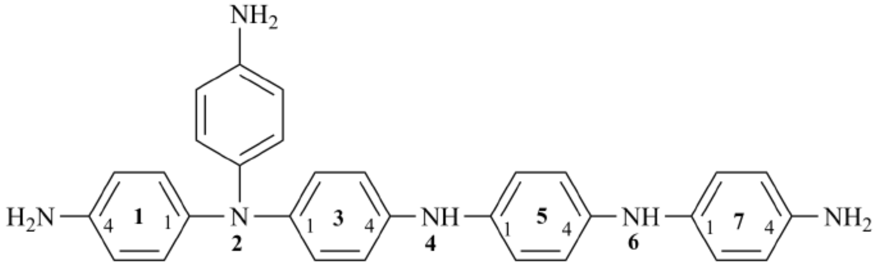
3,6,9,12-tetraazatetradecane-1,14-diamine (PIN)
(skeletal replacement ('a') name; see P-15.4)
*N*¹,*N*²-bis{2-[(2-aminoethyl)amino]ethyl}ethane-1,2-diamine (substitutive name)



*N*¹,*N*¹′-[1,4-phenylenedi(ethane-2,1-diyl)]di(propane-1,3-diamine) (PIN;
[multiplicative nomenclature (see P-15.3; P-51.3; P-62.2.5)
allows four amine characteristic groups to be included in the name)



*N*¹-(4-aminophenyl)-*N*⁴-phenylbenzene-1,4-diamine (PIN)
(maximum number of substituents cited as prefixes; see P-45.2.1)
[not *N*¹-(4-anilinophenyl)benzene-1,4-diamine]

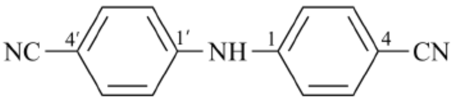


2-(4-aminophenyl)-2,4,6-triaza-1,7(1),3,5(1,4)-tetrabenzenaheptaphane-1^4,7^4-diamine (PIN)
(four benzene rings and a total of seven phane nodes justify a phane name; see P-52.2.5)
N^1,N^1-bis(4-aminophenyl)-N^4-{4-[(4-aminophenyl)amino]phenyl}benzene-1,4-diamine
(preferred substitutive name; maximum number of substituent prefixes)
N^1-(4-aminophenyl)-N^1,$N^{1'}$-[azanediyldi(4,1-phenylene)]di(benzene-1,4-diamine)
(multiplicative name; applicable only in general nomenclature)
N^4-[4-(4-aminoanilino)phenyl]-N^1,N^1-bis(4-aminophenyl)benzene-1,4-diamine

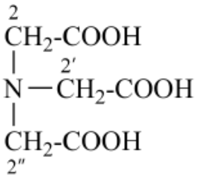
P-62.2.5 Multiplicative nomenclature

P-62.2.5.1 The prefixes 'nitrilo' for –N< and 'azanediyl' for –NH– (also written HN<) are recommended for use in multiplicative nomenclature (see P-15.3). The prefix 'imino' is reserved to denote only the divalent substituent group =NH. Multiplicative names are preferred to those formed by substitutive nomenclature when all conditions are fulfilled for the application of multiplicative nomenclature (see P-51.3).

Examples:



4,4′-azanediyldibenzonitrile (PIN)
4-[(4-cyanophenyl)amino]benzonitrile
4-(4-cyanoanilino)benzonitrile



$$\mathrm{N}(\overset{2}{\mathrm{C}}\mathrm{H_2\text{-}COOH})(\overset{2'}{\mathrm{C}}\mathrm{H_2\text{-}COOH})(\underset{2''}{\mathrm{C}}\mathrm{H_2\text{-}COOH})$$

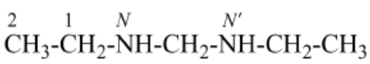
2,2′,2″-nitrilotriacetic acid
N,*N*-bis(carboxymethyl)glycine

P-62.2.5.2 Locants for nitrogen atoms in identical parent structures

The use of priming on the italic letter *N* to differentiate among different nitrogen atoms of parent structures requires special methods to indicate the attachment of identical parent structures to the multiplying substituent group through a nitrogen atom.

(1) Multiplied parent structures containing one nitrogen atom. The nitrogen atoms attached to the central substituent group are denoted by the symbols *N*, *N*′, *N*″, etc.

Example:



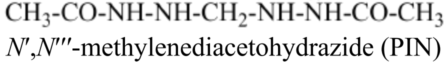
$$\overset{2}{\mathrm{CH_3}}\text{-}\overset{1}{\mathrm{CH_2}}\text{-}\overset{N}{\mathrm{NH}}\text{-}\mathrm{CH_2}\text{-}\overset{N'}{\mathrm{NH}}\text{-}\mathrm{CH_2}\text{-}\mathrm{CH_3}$$

N,*N*′-methylenediethanamine (PIN)
N,*N*′-diethylmethanediamine

(2) Multiplied parent structures containing two nitrogen atoms.

(i) The symbols *N*,*N*′ are used for the 'unprimed' parent structure and *N*″,*N*‴ for the 'primed parent structure'.

Example:



$$\mathrm{CH_3}\text{-}\mathrm{CO}\text{-}\overset{N''}{\mathrm{NH}}\text{-}\overset{N'''}{\mathrm{NH}}\text{-}\mathrm{CH_2}\text{-}\overset{N'}{\mathrm{NH}}\text{-}\overset{N}{\mathrm{NH}}\text{-}\mathrm{CO}\text{-}\mathrm{CH_3}$$

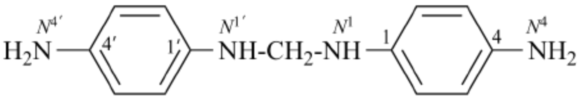
N′,*N*‴-methylenediacetohydrazide (PIN)

(ii) A combination of unprimed and primed numerical and letter locants is used as needed (see P-16.9.3). The numerical locant of the position on the parent structure at which the nitrogen atom is attached is cited as a superscript to the letter locant *N*, for example, N^1, $N^{1'}$, etc. A second identical parent structure has primed locants, i.e., 1′, 2′..., hence the nitrogen locant is $N^{1'}$.

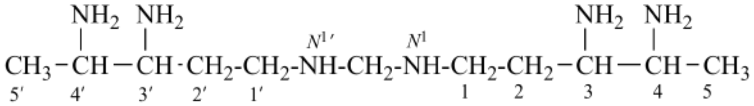
Examples:

$$\overset{N^{2'}}{H_2N}\text{-}\overset{2'}{CH_2}\text{-}\overset{1'}{CH_2}\text{-}\overset{N^{1'}}{NH}\text{-}CH_2\text{-}\overset{N^{1}}{NH}\text{-}\overset{1}{CH_2}\text{-}\overset{2}{CH_2}\text{-}\overset{N^{2}}{NH_2}$$

N^1,*N*$^{1'}$-methylenedi(ethane-1,2-diamine) (PIN)



N^1,*N*$^{1'}$-methylenedi(benzene-1,4-diamine) (PIN)

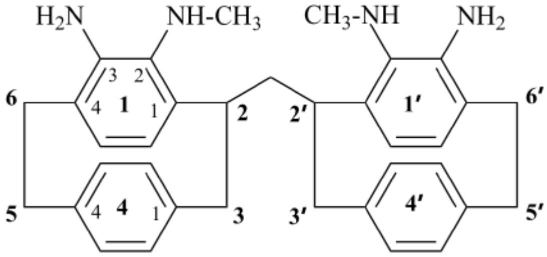


$$\underset{5'}{CH_3}-\underset{4'}{\overset{NH_2}{CH}}-\underset{3'}{\overset{NH_2}{CH}}\cdot\underset{2'}{CH_2}\text{-}\underset{1'}{CH_2}\text{-}\overset{N^{1'}}{NH}\text{-}CH_2\text{-}\overset{N^{1}}{NH}\text{-}\underset{1}{CH_2}\text{-}\underset{2}{CH_2}-\underset{3}{\overset{NH_2}{CH}}-\underset{4}{\overset{NH_2}{CH}}-\underset{5}{CH_3}$$

N^1,*N*$^{1'}$-methylenedi(pentane-1,3,4-triamine) (PIN)

P-62.2.5.3 For parent structures with multiple nitrogen atoms, such as di- or tricarboximidamides (see P-66.4), and cyclophanamines, even more complicated locant structures are required, such as primed letter locants with superscript numbers or with superscripted superscript numbers.

Example:



2,2′-methylenebis[*N*$^{1^2}$-methyl-1,4(1,4)dibenzenacyclohexaphane-1^2,1^3-diamine] (PIN)

P-62.2.6 Modification of the degree of saturation/unsaturation of amines

P-62.2.6.1 General methodology

When there is a choice for numbering, the starting point and the direction of numbering of a compound are chosen so as to give lowest locants to the following structural features (if present) considered successively in the order given until a decision is reached (see also P-14.4).

(a) fixed numbering (naphthalene, bicyclo[2.2.2]octane, etc.);

(b) heteroatoms in heterocycles and in acyclic parent structures;

(c) indicated hydrogen [for unsubstituted compounds; a higher locant may be needed at another position to provide for a substituent suffix in accordance with the structural feature (d)];

(d) principal group named as suffix;

(e) added indicated hydrogen (consistent with the structure of the compound and in accordance with further substitution);

(f) saturation/unsaturation (‘hydro’/‘dehydro’ prefixes) or unsaturation (‘ene’, ‘yne’ endings);

(g) substituents named as prefixes (low locants are allocated for substituents regardless of kind; then, if necessary, in the order of citation).

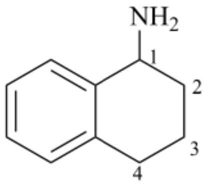
P-62.2.6.2 Modification of the degree of saturation/unsaturation of primary amines

Criteria (d), (e) and (f) described in the general methodology (P-62.2.6.1) are used.

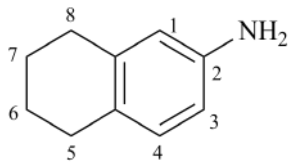
Examples:

$$\overset{3}{CH_2}{=}\overset{2}{CH}\text{-}\overset{1}{CH_2}\text{-}NH_2$$

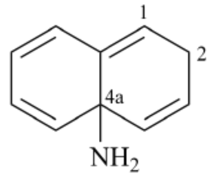
prop-2-en-1-amine (PIN)
(prop-2-en-1-yl)azane
allylamine



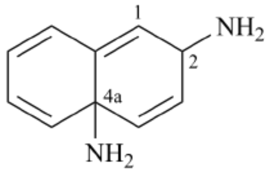
1,2,3,4-tetrahydronaphthalen-1-amine (PIN)
(1,2,3,4-tetrahydronaphthalen-1-yl)azane
(1,2,3,4-tetrahydronaphthalen-1-yl)amine



5,6,7,8-tetrahydronaphthalen-2-amine (PIN)
(5,6,7,8-tetrahydronaphthalen-2-yl)azane
(5,6,7,8-tetrahydronaphthalen-2-yl)amine



naphthalen-4a(2*H*)-amine (PIN)
(naphthalen-4a(2*H*)-yl)azane (naphthalen-4a(2*H*)-yl)amine



naphthalene-2,4a(2*H*)-diamine (PIN)
2,4a-dihydronaphthalene-2,4a-bis(azane) (see P-58.2)
2,4a-dihydronaphthalene-2,4a-diamine (see P-58.2)
naphthalene-2,4a(2*H*)-bis(azane)

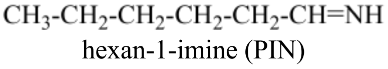
P-62.3 IMINES

Imines are characterized by a double bond between a carbon atom and a nitrogen atom. Thus, *N*-substituted imines, R-CH=N-R′ or R(R′)C=N-R″, must be classified as imines and not as amines in spite of the fact that there is a single bond between a carbon atom and the nitrogen atom; amines must have three single bonds linked to at least one carbon atom (see P-62.1). Imines must have a double bond between a carbon atom and the nitrogen. Compounds having the general structure R-CH=NR′ or R(R′)C=NR″ are called generically ‘aldimines’ and ‘ketimines’, respectively.

P-62.3.1 Substitutive names for imines

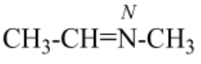
P-62.3.1.1 All imines are named substitutively using the suffix ‘imine’; the presence of several ‘imine’ characteristic groups is denoted by the numerical multiplying prefixes ‘di’, ‘tri’, etc. When there is a choice for numbering, the methodology described in P-62.2.4 for amines is recommended to generate preferred IUPAC names

Examples:



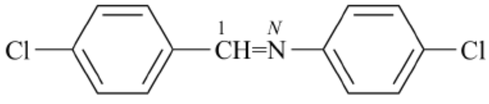
$$\overset{6}{\mathrm{CH_3}}\text{-}\overset{5}{\mathrm{CH_2}}\text{-}\overset{4}{\mathrm{CH_2}}\text{-}\overset{3}{\mathrm{CH_2}}\text{-}\overset{2}{\mathrm{CH_2}}\text{-}\overset{1}{\mathrm{CH}}{=}\overset{N}{\mathrm{NH}}$$

hexan-1-imine (PIN)

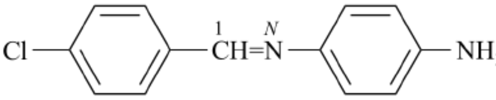


$$\mathrm{CH_3\text{-}CH}{=}\overset{N}{\mathrm{N}}\text{-}\mathrm{CH_3}$$

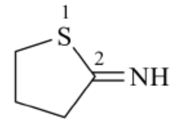
N-methylethanimine (PIN)
[not *N*-ethylidenemethanamine;
nor *N*-ethylidene(methyl)amine]



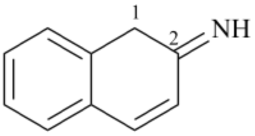
N,1-bis(4-chlorophenyl)methanimine (PIN)
(cf. the following example)



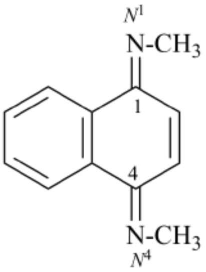
4-{[(4-chlorophenyl)methylidene]amino}aniline (PIN)



thiolan-2-imine (PIN)



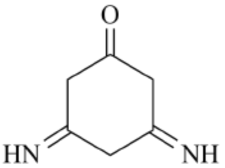
naphthalen-2(1*H*)-imine (PIN)
1,2-dihydronaphthalen-2-imine (see P-58.2.5)



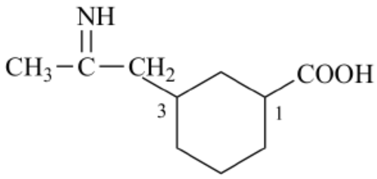
N^1,N^4-dimethylnaphthalene-1,4-diimine (PIN; see also P-16.9.2)
N,*N*′-dimethylnaphthalene-1,4-diimine (see also P-58.2.2.3)
N,*N*′-dimethyl-1,4-dihydronaphthalene-1,4-diimine
[not *N*,*N*′-dimethyl-1,4-naphthoquinone diimine;
two suffixes of different kinds are incompatible]
[not *N*,*N*′-(naphthalene-1,4-diylidene)bis(methanamine)]
[not *N*,*N*′-(naphthalene-1,4-diylidene)bis(methylamine)]
[not dimethyl(naphthalene-1,4-diylidene)bis(amine)]

P-62.3.1.2 The prefix ‘imino’ for =NH is used in presence of characteristic groups having seniority over imines. In multiplicative nomenclature, the prefix ‘azanylylidene’ is used for –N=. Substituent groups attached to rings, ring systems or heteroatoms of the type R-(C=NH)–, where R– is a ring or a chain, are named as acyl groups (see imidic acids, P-65.1.3.1 and acyl groups P-65.2).

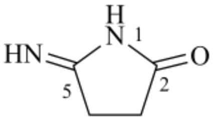
Examples:



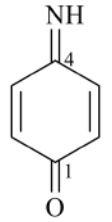
3,5-diiminocyclohexan-1-one (PIN)



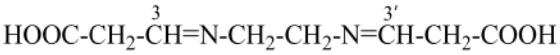
3-(2-iminopropyl)cyclohexane-1-carboxylic acid (PIN)



5-iminopyrrolidin-2-one (PIN)
(not 5-imino-2-pyrrolidone)

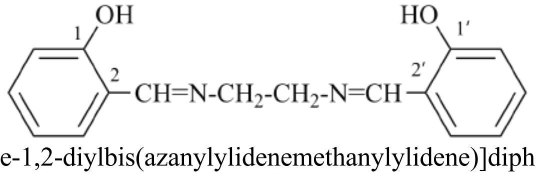


4-iminocyclohexa-2,5-dien-1-one (PIN)
(not *p*-benzoquinone monoimine)



$$\mathrm{HOOC\text{-}CH_2\text{-}\overset{3}{C}H{=}N\text{-}CH_2\text{-}CH_2\text{-}N{=}\overset{3'}{C}H\text{-}CH_2\text{-}COOH}$$

3,3′-[ethane-1,2-diylbis(azanylylidene)]dipropanoic acid (PIN)



2,2′-[ethane-1,2-diylbis(azanylylidenemethanylylidene)]diphenol (PIN)

P-62.3.1.3 Imino groups attached to heteroatoms (heteroimines)

Compounds containing the group X=NH, where X is a heteroatom and =NH the principal characteristic group, are named as imines; the prefix ‘imino’ is used to express the =NH group when another characteristic group has seniority over imines.

Examples:

$\mathrm{CH_3\text{-}P{=}NH}$
1-methylphosphanimine (PIN)

$\mathrm{(CH_3)_2Si{=}N\text{-}C_6H_5}$
1,1-dimethyl-*N*-phenylsilanimine (PIN)
(silane is a preselected name, see P-12.2)

$\mathrm{CH_3\text{-}N{=}SiH\text{-}CH_2\text{-}CO\text{-}O\text{-}CH_3}$
methyl [(methylimino)silyl]acetate (PIN)
(silyl is a preselected prefix, see P-12.2)

P-62.3.1.4 Carbodiimides

The hypothetical compound HN=C=NH is named systematically ‘methanediimine’. Its derivatives are named as substitution products thereof. These names are preferred to those based on the retained name ‘carbodiimide’, which now should be used only as a class name.

Example:

$\mathrm{C_6H_{11}\text{-}N{=}C{=}N\text{-}C_6H_{11}}$
dicyclohexylmethanediimine (PIN)
(formerly dicyclohexylcarbodiimide)

P-62.4 *N*-SUBSTITUTION OF AMINES AND IMINES BY HETEROATOMS

Traditionally, substitution on the nitrogen atom of amines and imines was allowed for all characteristic groups cited as prefixes (see Table 5.1). This approach is maintained in these recommendations, unless a higher class is formed that must be named in accordance with the seniority of classes (see P-41).

This new rule is applied to prefixes such as Cl and other halogen atoms, –BrO and other acyl similar groups, –NO, $\mathrm{–NO_2}$, –OR, $\mathrm{–SO_2\text{-}R}$, –SO-R, and even –OH groups and chalcogen analogues.

> This is a change. In accordance with the seniority of classes (see P-41), compounds such as R-NH-Cl, R-NH-NO, and $\mathrm{R\text{-}NH\text{-}NO_2}$ are now named as derivatives of amides (see P-67.1.2.6). Compounds such as R-NH-OH are named as *N*-derivatives of the senior amine (see P-68.3.1.1.1).

Substitution of amines is permitted by –OR , –SR, –SeR, and –TeR groups, where R is an alkyl or aryl substituent group.

Examples:

$\mathrm{CH_3\text{-}CH_2\text{-}NH\text{-}O\text{-}CH_3}$
N-methoxyethanamine (PIN, see P-68.3.1.1.1.3)

$CH_3\text{-}CH_2\text{-}NH\text{-}OH$
N-hydroxyethanamine (PIN)
N-ethylhydroxylamine

$CH_3\text{-}CH_2\text{-}\overset{N}{N}H\text{-}Cl$
ethylhypochlorous amide (PIN)
N-chloroethanamine

$CH_3\text{-}\overset{N}{N}H\text{-}NO$
methylnitrous amide (PIN)
N-nitrosomethanamine

$CH_3\text{-}N(NO_2)_2$
methyl(nitro)nitramide (PIN)
N,*N*-dinitromethanamine

$CH_3\text{-}NH\text{-}BrO$
methylbromous amide (PIN)
N-bromosylmethanamine

P-62.5 AMINE OXIDES, IMINE OXIDES, AND CHALCOGEN ANALOGUES

Amine oxides, imine oxides, and their chalcogen analogues are named:

(1) by functional class nomenclature using the class names ‘oxide’, ‘sulfide’, ‘selenide’, and ‘telluride’ provided that unambiguous superscripted *N* locants can be used, if necessary ;

(2) by use of prefixes derived from the parent name λ^5-azane;

(3) as zwitterions (see P-74.2.1.2).

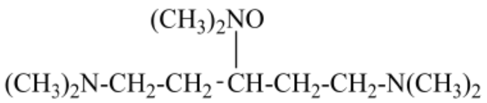
Method (1) is used when one amine or imine oxide is present. Because of the zwitterionic nature of a nitrogen oxide, amine and imine oxides are placed with zwitterions in the order of compound classes (see P-41). Thus, amine and imine oxides are named by method (1) and all other amino groups, if present, are named as substituent groups by using the prefix ‘amino’. Method (2) is used when the oxide is on a nitrogen atom of a substituent group; the locant *N* is used before the term ‘oxide’ when locants are present in the name of the amine.

Method (1) or (2), as appropriate, leads to preferred IUPAC names as illustrated below. Names of zwitterions are described in P-74.2.1.2.

Examples:

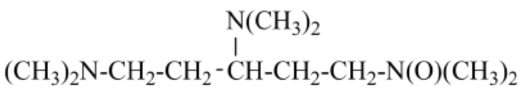
$(CH_3)_3NO$ or $(CH_3)_3N^+\text{-}O^-$
(1) *N*,*N*-dimethylmethanamine *N*-oxide (PIN)
(trimethyl)amine oxide
(3) (trimethylazaniumyl)oxidanide (see P-74.2.1.2)

$CH_2{=}N(O)Cl$
(1) *N*-chloromethanimine *N*-oxide (PIN)
(3) [chloro(methylidene)azaniumyl]oxidanide (see also P-74.2.1.2)



$$(CH_3)_2N\text{-}CH_2\text{-}CH_2\text{-}\overset{\overset{\displaystyle (CH_3)_2NO}{|}}{C}H\text{-}CH_2\text{-}CH_2\text{-}N(CH_3)_2$$

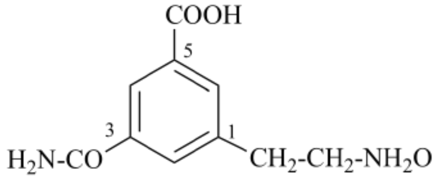
1,5-bis(dimethylamino)-*N*,*N*-dimethylpentan-3-amine *N*-oxide (PIN)
(not N^1,N^1,N^3,N^3,N^5,N^5-hexamethylpentane-1,3,5-triamine N^3-oxide;
the *N*-oxide is classified as a zwitterion and it is the preferred characteristic group)



$$(CH_3)_2N\text{-}CH_2\text{-}CH_2\text{-}\overset{\overset{\displaystyle N(CH_3)_2}{|}}{C}H\text{-}CH_2\text{-}CH_2\text{-}N(O)(CH_3)_2$$

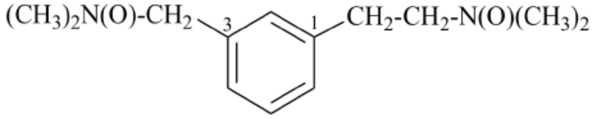
3,5-bis(dimethylamino)-*N*,*N*-dimethylpentan-1-amine *N*-oxide (PIN)
(not N^1,N^1,N^3,N^3,N^5,N^5-hexamethylpentane-1,3,5-triamine N^1-oxide;
the *N*-oxide is classified as a zwitterion and it is the preferred characteristic group)

$(CH_3)_2N\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}N(O)(CH_3)_2$
5-(dimethylamino)-*N*,*N*-dimethylpentane-1-amine *N*-oxide (PIN)
(not N^1,N^1,N^5,N^5-tetramethylpentane-1,5-diamine N^1-oxide;
the *N*-oxide is classified as a zwitterion and it is the preferred characteristic group)



(1) 2-(3-carbamoyl-5-carboxyphenyl)ethan-1-amine *N*-oxide (PIN)
3-(2-aminoethyl)-5-carbamoylbenzoic acid N^3-oxide
(3) {[2-(3-carbamoyl-5-carboxyphenyl)ethyl]azaniumyl}oxidanide (see also P-74.2.1.2)

$\bullet CH_2\text{-}CH_2\text{-}NH_2O$
(2) 2-(oxo-λ^5-azanyl)ethyl (PIN)
(3) 2-(oxidoazaniumyl)ethyl



(2) 2-(3-{[dimethyl(oxo)-λ^5-azanyl]methyl}phenyl)-*N*,*N*-dimethylethan-1-amine *N*-oxide (PIN)
2-{3-[(dimethylamino)methyl]phenyl}-*N*,*N*-dimethylethan-1-amine N^1,N^3-dioxide
(3) 2-(3-{[dimethyl(oxido)azaniumyl]methyl}phenyl)-*N*,*N*-dimethylethan-1-amine *N*-oxide
(see also P-74.2.1.2)

$(CH_3\text{-}CH_2)_3NS$
(1) *N*,*N*-diethylethanamine *N*-sulfide (PIN)
(triethyl)amine sulfide
(3) (triethylazaniumyl)sulfanide (see also P-74.2.1.2)

P-62.6 AMINE AND IMINE SALTS

P-62.6.1 Cation and anion names

Salts of tetravalent nitrogen $R_4N^+\ X^-$ (where one R group represents the parent hydride of the amine or imine and the other groups are hydrogen atoms or substituent groups) are named by one of the following methods:

(1) by adding the suffix ‘ium’ to the name of the amine or imine, with elision of the terminal letter ‘e’, if present, substituent groups being cited as prefixes, and the name of the anion added as a separate word;

(2) by substituting the parent hydride ‘azanium’, NH_4^+;

(3) by substituting the parent hydride ‘ammonium’, NH_4^+, for quaternary salts only.

Method (1) leads to preferred IUPAC names.

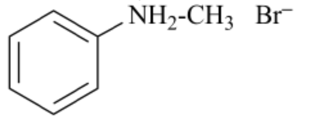
Examples:

$CH_3\text{-}\overset{+}{N}H_3\ \ Cl^-$
(1) methanaminium chloride (PIN)
(2) methylazanium chloride

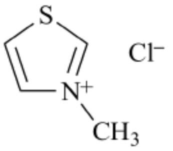
$CH_3\text{-}CH_2\text{-}\overset{+}{N}H_2\text{-}CH_3\ \ Br^-$
(1) *N*-methylethanaminium bromide (PIN)
(2) ethyl(methyl)azanium bromide

$CH_3\text{-}CH_2\text{-}\overset{+}{N}H(CH_3)_2\ \ I^-$
(1) *N*,*N*-dimethylethanaminium iodide (PIN)
(2) ethyldi(methyl)azanium iodide

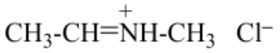
$(CH_3)_4N^+\ I^-$
(1) *N*,*N*,*N*-trimethylmethanaminium iodide (PIN)
(2) tetramethylazanium iodide
(3) tetramethylammonium iodide



(1) *N*-methylanilinium bromide (PIN)
N-methylbenzenaminium bromide
(2) methyl(phenyl)azanium bromide

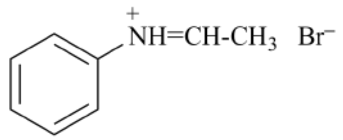


(1) 3-methyl-1,3-thiazol-3-ium chloride (PIN)



$CH_3\text{-}CH\text{=}\overset{+}{N}H\text{-}CH_3 \quad Cl^-$

(1) *N*-methylethaniminium chloride (PIN)
(2) ethylidene(methyl)azanium chloride

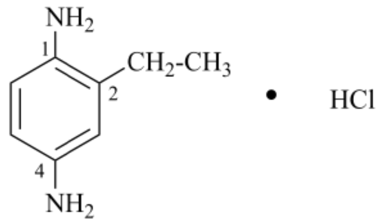


(1) *N*-phenylethaniminium bromide (PIN)
(2) ethylidene(phenyl)azanium bromide

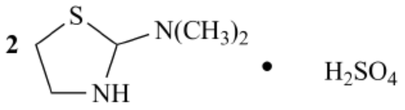
P-62.6.2 Salts of indefinite structure (adducts)

When the above rule cannot be applied because the structure is indefinite, amine and imine salts are named as organic-inorganic adducts, see P-14.8.2. Formulas for these adducts are written as described in P-14.8. Names are constructed in the order that the formulas are written. Preferred IUPAC names cannot be assigned to salts that include inorganic acids pending the development of rules for choosing preferred IUPAC names for inorganic substances.

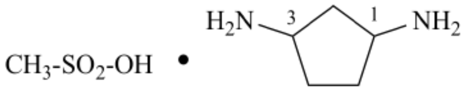
Examples:



2-ethylbenzene-1,4-diamine—hydrogen chloride (1/1)



N,*N*-dimethyl-1,3-thiazolidin-2-amine—sulfuric acid (2/1)



methanesulfonic acid—cyclopentane-1,3-diamine (1/1) (PIN)

P-63 HYDROXY COMPOUNDS, ETHERS, PEROXOLS, PEROXIDES, AND CHALCOGEN ANALOGUES

P-63.0 Introduction
P-63.1 Hydroxy compounds and chalcogen analogues
P-63.2 Ethers and chalcogen analogues
P-63.3 Peroxides and chalcogen analogues
P-63.4 Hydroperoxides (peroxols) and chalcogen analogues
P-63.5 Cyclic ethers, sulfides, selenides, and tellurides
P-63.6 Sulfoxides and sulfones
P-63.7 Polyfunctional compounds
P-63.8 Salts of hydroxy compounds, hydroperoxy compounds and their chalcogen analogues

P-63.0 INTRODUCTION

Traditionally, hydroxy compounds are compounds having one or more hydroxy groups attached to carbon atoms. Alcohols, phenols, ‘enols’ and ‘ynols’ are recognized as important classes of hydroxy compounds. The category is extended so as to include compounds having one or more hydroxy groups attached to atoms other than carbon without being classified as acids as defined in the seniority of classes. For instance, $H_3Si\text{-}OH$ is classified and named as a hydroxy compound, silanol, but $Si(OH)_4$ is classified and named as an acid, silicic acid.

The suffix ‘peroxol’ is now introduced to name the group –OOH, formerly named by functional class nomenclature as ‘hydroperoxide’. Chalcogen analogues are names by suffixes such as ‘thioperoxol’, ‘dithioperoxol’, ‘selenoperoxol’, and ‘selenothioperoxol’.

Rules on hydroxy compounds (alcohols and phenols), ethers, hydroperoxides, peroxides, and their chalcogen analogues, discussed as Rules C-201 to C-218 in the 1979 Recommendations (ref. 1) and Rule R-5.5 in the 1993 Recommendations (ref. 2) are superseded by the corresponding rules described in this section, P-63.

P-63.1 HYDROXY COMPOUNDS AND CHALCOGEN ANALOGUES

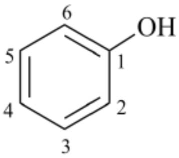
Names generated substitutively are preferred IUPAC names rather than functional class names or retained names, with the exception of the retained name 'phenol' that can be fully substituted. Functional class names are traditional names that are restricted today to alcohols, R-OH, where the R– group is a simple aliphatic or alicyclic group.

P-63.1.1 Retained names
P-63.1.2 Systematic names of alcohols, phenols, enols, and ynols
P-63.1.3 Heterols
P-63.1.4 Substitutive nomenclature, prefix mode
P-63.1.5 Sulfur, selenium and tellurium analogues of hydroxy compounds

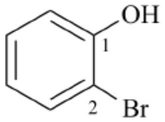
P-63.1.1 Retained names

P-63.1.1.1 Only one name is retained, phenol, for C_6H_5-OH, both as a preferred name and for general nomenclature. The structure is substitutable at any position. Locants 2, 3, and 4 are recommended, not *o*, *m*, and *p*.

Examples:



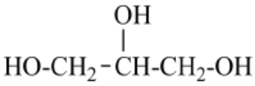
phenol (PIN; retained name)



2-bromophenol (PIN)
(not *o*-bromophenol)

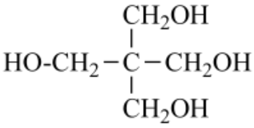
P-63.1.1.2 The following names are retained but only for general nomenclature and only when unsubstituted.

HO-CH_2-CH_2-OH
ethylene glycol
ethane-1,2-diol (PIN)



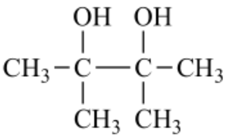
$$\mathrm{HO{-}CH_2{-}\overset{\displaystyle OH}{\overset{|}{C}}H{-}CH_2{-}OH}$$

glycerol
propane-1,2,3-triol (PIN)



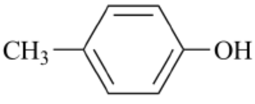
$$\mathrm{HO{-}CH_2{-}\underset{\underset{\displaystyle CH_2OH}{|}}{\overset{\overset{\displaystyle CH_2OH}{|}}{C}}{-}CH_2OH}$$

pentaerythritol
2,2-bis(hydroxymethyl)propane-1,3-diol (PIN)

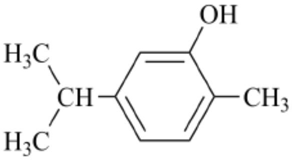


$$\mathrm{CH_3{-}\underset{\underset{\displaystyle CH_3}{|}}{\overset{\overset{\displaystyle OH}{|}}{C}}{-}\underset{\underset{\displaystyle CH_3}{|}}{\overset{\overset{\displaystyle OH}{|}}{C}}{-}CH_3}$$

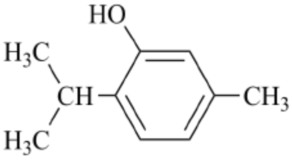
pinacol
2,3-dimethylbutane-2,3-diol (PIN)



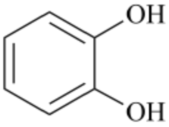
cresol (*p*-isomer shown ; also *o*- and *m*-isomers)
4-methylphenol (PIN)



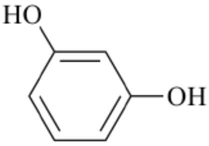
carvacrol
2-methyl-5-(propan-2-yl)phenol (PIN)



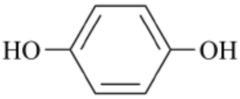
thymol
5-methyl-2-(propan-2-yl)phenol (PIN)



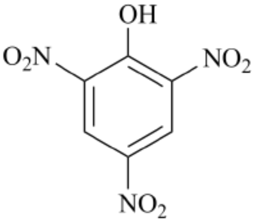
pyrocatehol
benzene-1,2-diol (PIN)



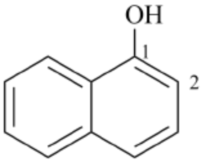
resorcinol
benzene-1,3-diol (PIN)



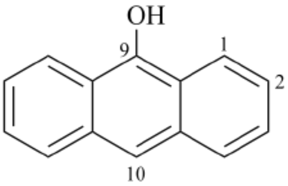
hydroquinone
benzene-1,4-diol (PIN)



picric acid
2,4,6-trinitrophenol (PIN)



1-naphthol
naphthalen-1-ol (PIN)



9-anthrol
anthracen-9-ol (PIN)

P-63.1.2 Systematic names of alcohols, phenols, enols, and ynols

Hydroxy compounds are named in three ways:

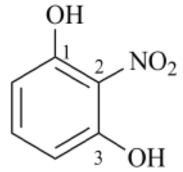
(1) substitutively, using the suffix ‘ol’ and the prefix ‘hydroxy’. The presence of several ‘ol’ characteristic groups is denoted by the numerical multiplying prefixes ‘di’, ‘tri’, etc.; the final letter ‘a’ in a multiplying prefix is elided before the suffix ‘ol’. Rule P-44 is applied when a principal chain or a senior ring system must be chosen. When there is a choice for numbering, the starting point and the direction of numbering of a compound are chosen so as to give lowest locants to the ‘ol’ suffixes;

(2) by functional class nomenclature and the class term ‘alcohol’;

(3) as assemblies of identical units by multiplicative nomenclature when the conditions for its use are fulfilled (see P-51.3)

Method (1) generates preferred IUPAC names. Names as assemblies of identical units, method (3), are preferred to those that are formed by simple substitution (P-51.1.5).

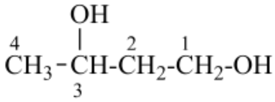
Examples:



(1) 2-nitrobenzene-1,3-diol (PIN)
(not 2-nitroresorcinol)

CH_3-OH
(1) methanol (PIN)
(2) methyl alcohol

$(CH_3)_3C$-OH
(1) 2-methylpropan-2-ol (PIN)
(2) *tert*-butyl alcohol

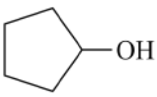


$$\overset{4}{C}H_3\text{-}\underset{3}{\overset{OH}{C}}H\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}H_2\text{-}OH$$

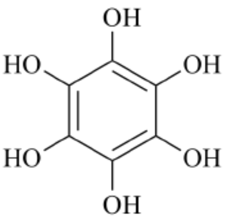
(1) butane-1,3-diol (PIN)

$$HO\text{-}\overset{5}{C}H_2\text{-}\overset{4}{C}H_2\text{-}\overset{3}{C}H\text{=}\overset{2}{C}H\text{-}\overset{1}{C}H_2\text{-}OH$$

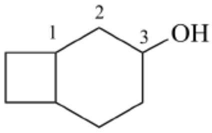
(1) pent-2-ene-1,5-diol (PIN)



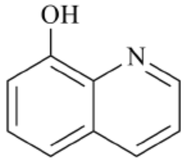
(1) cyclopentanol (PIN)



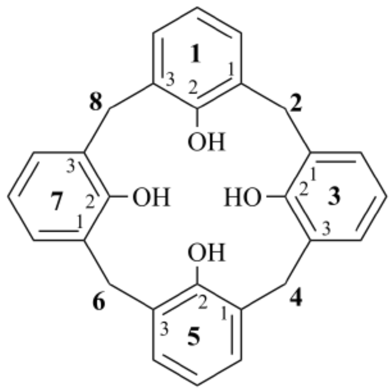
(1) benzenehexol (PIN)



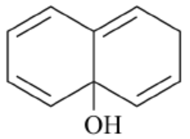
(1) bicyclo[4.2.0]octan-3-ol (PIN)



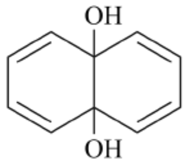
(1) quinolin-8-ol (PIN)


1
8
2
OH
7
OH
HO
3
OH
6
4
5

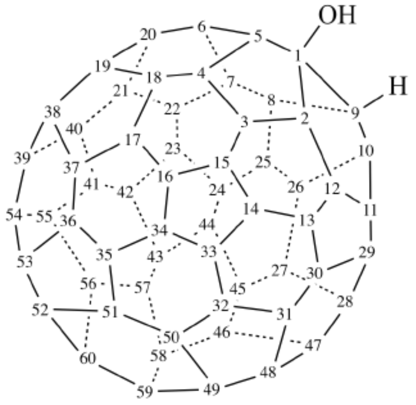
1,3,5,7(1,3)-tetrabenzenacyclooctaphane-$1^2,3^2,5^2,7^2$-tetrol (PIN)



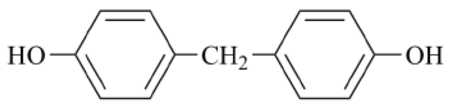
(1) naphthalen-4a(2*H*)-ol (PIN)
2,4a-dihydronaphthalen-4a-ol
(see P-58.2)



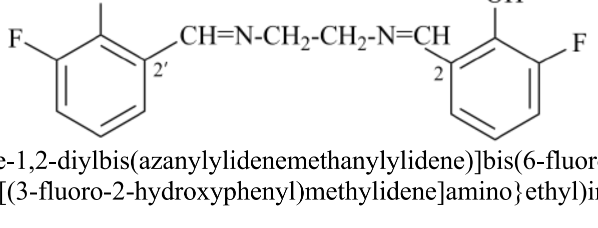
(1) naphthalene-4a,8a-diol (PIN)
4a,8a-dihydronaphthalene-4a,8a-diol
(see P-58.2)



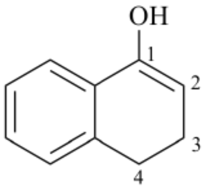
(C_{60}-I_h)[5,6]fulleren-1(9*H*)-ol (PIN)
1,9-dihydro(C_{60}-I_h)[5,6]fulleren-1-ol
(see P-58.2)



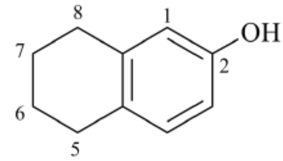
(3) 4,4′-methylenediphenol (PIN)
(1) 4-[(4-hydroxyphenyl)methyl]phenol


OH
F
CH=N-CH2-CH2-N=CH
2′
OH
F
2

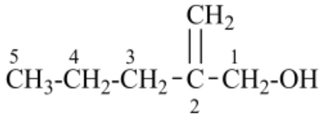
(3) 2,2′-[ethane-1,2-diylbis(azanylylidenemethanylylidene)]bis(6-fluorophenol)(PIN)
(1) 2-fluoro-6-{[(2-{[(3-fluoro-2-hydroxyphenyl)methylidene]amino}ethyl)imino]methyl}phenol



(1) 3,4-dihydronaphthalen-1-ol (PIN)

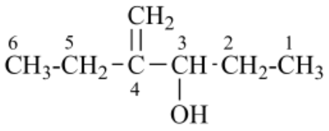


(1) 5,6,7,8-tetrahydronaphthalen-2-ol (PIN)



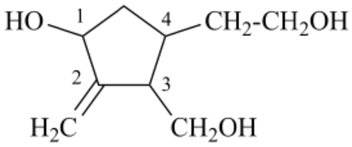
$$\overset{5}{CH_3}\text{-}\overset{4}{CH_2}\text{-}\overset{3}{CH_2}\text{-}\underset{2}{\overset{\overset{CH_2}{\|}}{C}}\text{-}\overset{1}{CH_2}\text{-}OH$$

(1) 2-methylidenepentan-1-ol (PIN)

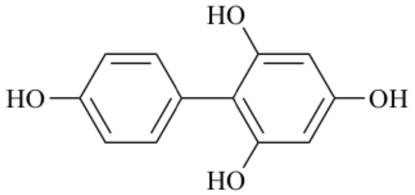


$$\overset{6}{CH_3}\text{-}\overset{5}{CH_2}\text{-}\underset{4}{\overset{\overset{CH_2}{\|}}{C}}\text{-}\underset{\underset{OH}{|}}{\overset{3}{CH}}\text{-}\overset{2}{CH_2}\text{-}\overset{1}{CH_3}$$

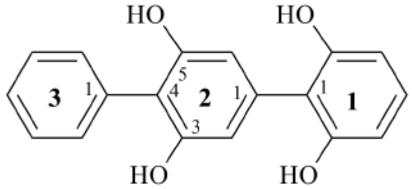
(1) 4-methylidenehexan-3-ol (PIN)


HO
1
4
CH2-CH2OH
2
3
H2C
CH2OH

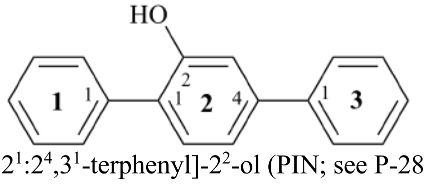
(1) 4-(2-hydroxyethyl)-3-(hydroxymethyl)-2-methylidenecyclopentan-1-ol (PIN)



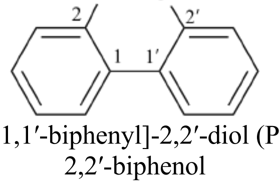
(1) [1,1′-biphenyl]-2,4,4′,6-tetrol (PIN)
biphenyl-2,4,4′,6-tetrol


HO
HO
3
1
5
4
2
1
1
1
3
HO
HO

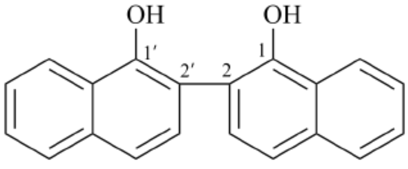
(1) [1^1,2^1:2^4,3^1-terphenyl]-1^2,1^6,2^3,2^5-tetrol (PIN)
(in the PIN brackets enclose the name of an assembly requiring
locants when suffixes are present; for numbering, see P-28.3)
[1,1′:4′,1″-terphenyl]-2,3′,5′,6-tetrol (see P-28.3)


HO
2
1
1
1
2
4
1
3

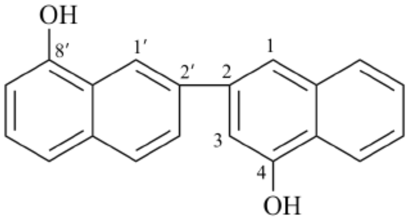
[1^1,2^1:2^4,3^1-terphenyl]-2^2-ol (PIN; see P-28.3]
[1,1′:4′,1″-terphenyl]-2′-ol (see P-28.3)



(1) [1,1′-biphenyl]-2,2′-diol (PIN)
2,2′-biphenol



[2,2′-binaphthalene]-1,1′-diol (PIN)
2,2′-bi-1-naphthol



(1) [2,2′-binaphthalene]-4,8′-diol (PIN)
3,7′-bi-1-naphthol

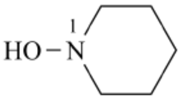
P-63.1.3 Heterols

When the hydroxy group is attached to an atom other than carbon, hydroxy compounds belong to a compound class called heterols. They are classified as hydroxy compounds and named using the suffix ‘ol’, unless they are classified as acids and denoted by a retained name. Names formed using a suffix are preferred to those formed by means of the prefix ‘hydroxy’.

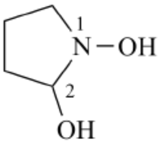
Examples:

$(CH_3)_3Si\text{-}OH$
trimethylsilanol (PIN)
hydroxytri(methyl)silane
(silane is a preselected name; see P-12.2)

$(CH_3\text{-}CH_2)_2AlOH$
diethylalumanol
diethyl(hydroxy)alumane
(alumane is a preselected name; see P-12.2)



piperidin-1-ol (PIN)
1-hydroxypiperidine
N-hydroxypiperidine



pyrrolidine-1,2-diol (PIN)
1-hydroxypyrrolidin-2-ol
N-hydroxypyrrolidin-2-ol

$P(OH)_3$
phosphorous acid (retained preselected name)
(not phosphanetriol)

$H_2As\text{-}OH$
arsinous acid (retained preselected name)
(not arsanol)

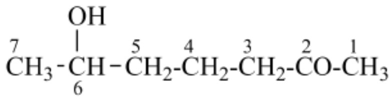
P-63.1.4 Substitutive nomenclature, prefix mode

Hydroxy groups are indicated by the prefix ‘hydroxy’ when:

(1) a group having priority for citation as the principal characteristic group is present; or

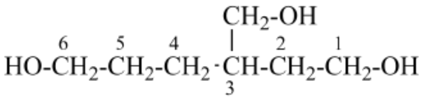
(2) a hydroxy group cannot be denoted by a suffix.

Examples:



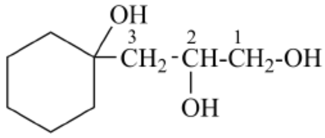
$$\overset{7}{\mathrm{C}}\mathrm{H_3}\text{-}\underset{6}{\overset{\overset{\mathrm{OH}}{|}}{\mathrm{C}}}\mathrm{H}\text{-}\overset{5}{\mathrm{C}}\mathrm{H_2}\text{-}\overset{4}{\mathrm{C}}\mathrm{H_2}\text{-}\overset{3}{\mathrm{C}}\mathrm{H_2}\text{-}\overset{2}{\mathrm{C}}\mathrm{O}\text{-}\overset{1}{\mathrm{C}}\mathrm{H_3}$$

(1) 6-hydroxyheptan-2-one (PIN)

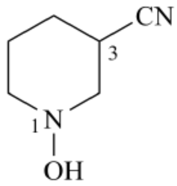


$$\mathrm{HO}\text{-}\overset{6}{\mathrm{C}}\mathrm{H_2}\text{-}\overset{5}{\mathrm{C}}\mathrm{H_2}\text{-}\overset{4}{\mathrm{C}}\mathrm{H_2}\text{-}\underset{3}{\overset{\overset{\mathrm{CH_2\text{-}OH}}{|}}{\mathrm{C}}}\mathrm{H}\text{-}\overset{2}{\mathrm{C}}\mathrm{H_2}\text{-}\overset{1}{\mathrm{C}}\mathrm{H_2}\text{-}\mathrm{OH}$$

(2) 3-(hydroxymethyl)hexane-1,6-diol (PIN)



(2) 3-(1-hydroxycyclohexyl)propane-1,2-diol (PIN)



(1) 1-hydroxypiperidine-3-carbonitrile (PIN)

$$\mathrm{HO\text{-}PH}\text{-}\overset{3}{\mathrm{C}}\mathrm{H_2}\text{-}\overset{2}{\mathrm{C}}\mathrm{H_2}\text{-}\overset{1}{\mathrm{C}}\mathrm{OOH}$$

(1) 3-(hydroxyphosphanyl)propanoic acid (PIN)

P-63.1.5 Sulfur, selenium, and tellurium analogues of hydroxy compounds

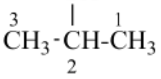
Sulfur, selenium, and tellurium analogues of hydroxy compounds are named substitutively using the suffixes ‘thiol’, ‘selenol’, and ‘tellurol’, and the prefixes ‘sulfanyl’, ‘selanyl’, and ‘tellanyl’, respectively; the presence of several of the same kind of ‘ol’ characteristic groups is denoted by the numerical multiplying prefixes ‘di’, ‘tri’, etc. The prefixes ‘mercapto’ (–SH), and ‘hydroseleno’ or selenyl (–SeH), etc. are no longer recommended.

Functional class nomenclature is not used.

Names of assemblies of identical units are formed by methods described in P-15.3 and P-51.3. Names for divalent prefixes are described in P-63.2.5. Multiplicative names are preferred to substitutive names when all conditions for their formation are fulfilled (P-51.1.5).

The seniority order of sulfur, selenium, and tellurium analogues of hydroxy compounds is: O > S > Se > Te.

Examples:



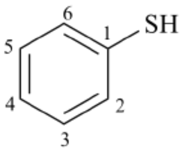
$$\overset{3}{\mathrm{C}}\mathrm{H_3}\text{-}\underset{2}{\overset{\overset{\mathrm{SH}}{|}}{\mathrm{C}}}\mathrm{H}\text{-}\overset{1}{\mathrm{C}}\mathrm{H_3}$$

propane-2-thiol (PIN)

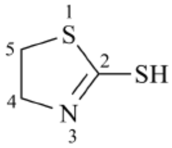
$CH_3\text{-}CH_2\text{-}SeH$
ethaneselenol (PIN)

$$\mathrm{HS}\text{-}\overset{4}{\mathrm{C}}\mathrm{H_2}\text{-}\overset{3}{\mathrm{C}}\mathrm{H_2}\text{-}\overset{2}{\mathrm{C}}\mathrm{H_2}\text{-}\overset{1}{\mathrm{C}}\mathrm{H_2}\text{-}\mathrm{SH}$$

butane-1,4-dithiol (PIN)



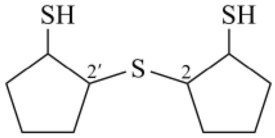
benzenethiol (PIN)
(not thiophenol)



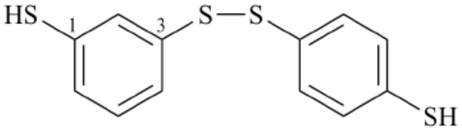
4,5-dihydro-1,3-thiazole-2-thiol (PIN)

$\text{HS-}\overset{3}{C}H_2\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}OOH$

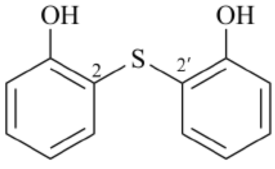
3-sulfanylpropanoic acid (PIN)



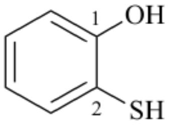
2,2′-sulfanediyldi(cyclopentane-1-thiol) (PIN)



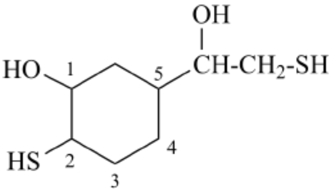
3-[(4-sulfanylphenyl)disulfanyl]benzene-1-thiol (PIN)
3,4′-disulfanediyldi(benzene-1-thiol)



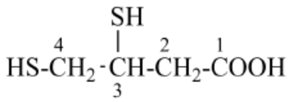
2,2′-sulfanediyldiphenol (PIN)
2-[(2-hydroxyphenyl)sulfanyl]phenol



2-sulfanylphenol (PIN)



5-(1-hydroxy-2-sulfanylethyl)-2-sulfanylcyclohexan-1-ol (PIN)
(ring preferred to chain, see P-52.2.8)
1-(3-hydroxy-4-sulfanylcyclohexyl)-2-sulfanylethan-1-ol



$\text{HS-}\overset{4}{C}H_2\text{-}\overset{SH}{\underset{3}{CH}}\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}OOH$

3,4-bis(sulfanyl)butanoic acid (PIN)

P-63.2 ETHERS AND CHALCOGEN ANALOGUES

P-63.2.1 Definitions and general methodology
P-63.2.2 Names of substituent groups R′-O–, R′-S–, R′-Se–, and R′-Te–
P-63.2.3 Retained names of ethers
P-63.2.4 Systematic names of ethers
P-63.2.5 Names of chalcogen analogues of ethers: i.e., sulfides, selenides, and tellurides

P-63.2.1 Definitions and general methodology

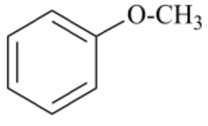
Ethers have the general formula R-O-R′, in which R = R′ or R ≠ R′; R and R′ can be any substituent group, aliphatic or cyclic, organyl (the free valence attached to a carbon atom) or organoheteryl (the free valence attached to an atom other than carbon), derived from the parent hydrides described in P-29.

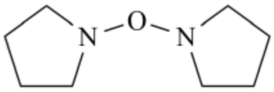
Examples:

$CH_3\text{-O-}CH_3$

$(CH_3)_3Si\text{-}O\text{-}CH_3$

$H_3Ge\text{-}O\text{-}GeH_3$





Chalcogen analogues are generically called sulfides, R-S-R′, selenides, R-Se-R′, and tellurides, R-Te-R′.

Names for ethers and their chalcogen analogues are formed by various methods in accordance with the principles of substitutive nomenclature, multiplicative nomenclature, skeletal replacement (‘a’) nomenclature, phane nomenclature, and functional class nomenclature. However, some ethers and chalcogen analogues are classified as parent hydrides and named as such, for example $H_3Ge\text{-}O\text{-}GeH_3$, digermoxane, and similar compounds described in Section P-21.2.3.1. These compounds are thus not named by the methods described in this Section, because their names are subject to selection rules with regard to heteroatom content.

In substitutive nomenclature, when R is different from R′, RH is chosen as parent hydride and R′-O– is cited as a substituent to it. Names of these substituent groups are described in Section P-63.2.2. Functional class nomenclature uses substituent group names for R and R′.

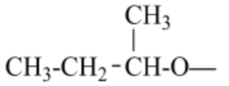
P-63.2.2 Names of substituent groups R′-O–, R′-S–, R′-Se–, and R′-Te–

P-63.2.2.1 Systematic names

P-63.2.2.1.1 Substituent prefix names for R′-O– groups are formed by concatenation, i.e., by adding the prefix ‘oxy’ to the substituent prefix name for the group R′. These compound prefixes require the numerical multiplying prefixes ‘bis’, ‘tris’, etc.

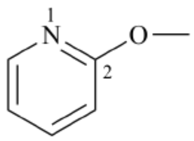
Examples:

$CH_3\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}O—$
pentyloxy (preferred prefix)

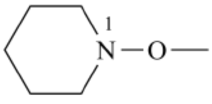


$CH_3\text{-}CH_2\text{-}\underset{}{\overset{CH_3}{\overset{|}{C}}}H\text{-}O—$

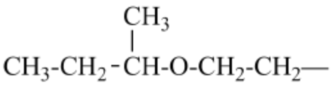
(butan-2-yl)oxy (preferred prefix)
1-methylpropoxy



(pyridin-2-yl)oxy (preferred prefix)
2-pyridyloxy



(piperidin-1-yl)oxy (preferred prefix)
piperidinooxy



$CH_3\text{-}CH_2\text{-}\overset{CH_3}{\overset{|}{C}}H\text{-}O\text{-}CH_2\text{-}CH_2—$

2-[(butan-2-yl)oxy]ethyl (preferred prefix)

$H_3Si\text{-}O—$
silyloxy (preselected prefix)
(not siloxy)

P-63.2.2.1.2 Substituent prefixes for the substituent groups R′S–, R′Se–, and R′Te–, are formed by substitution of the groups HS–, ‘sulfanyl’, HSe–, ‘selanyl’; and HTe–, ‘tellanyl’; they require the multiplicative prefixes ‘bis’, ‘tris’, etc. The former names ‘thio’, –S–; ‘seleno’, –Se–; and ‘telluro’, –Te– may be used as additive prefixes in general nomenclature.

Examples:

CH_3-S–
methylsulfanyl (preferred prefix)
methylthio

C_6H_5-Se–
phenylselanyl (preferred prefix)
phenylseleno

P-63.2.2.1.3 Divalent groups, such as –O-Y-O– or –S-Y-S–, are named by adding (concatenating) the prefixes ‘oxy’, ‘sulfanediyl’, etc. to the name of the divalent group Y. The multiplying prefix ‘bis’ is used in preferred names instead of ‘di’ to avoid ambiguity. Parentheses are used after the multiplying prefix ‘bis’, ‘tris’ etc., even around simple prefixes.

Examples:

–O-CH_2-O–
methylenebis(oxy) (preferred prefix)
(not methylenedioxy)

–S-CH_2-S–
methylenebis(sulfanediyl) (preferred prefix)

–CH_2-S-CH_2–
sulfanediylbis(methylene) (preferred prefix)
(not sulfanediyldimethylene)

P-63.2.2.2 Retained names

Some contracted names are retained for R-O– substituent groups. They are used both as preferred IUPAC prefixes and in general nomenclature; they are fully substitutable (with the exception of *tert*-butoxy) and are considered as simple prefixes requiring the numerical prefixes ‘di’, ‘tri’, etc. They are:

CH_3-O–
methoxy (preferred prefix)

CH_3-CH_2-O–
ethoxy (preferred prefix)

CH_3-$[CH_2]_2$-O–
propoxy (preferred prefix)

CH_3-$[CH_2]_3$-O–
butoxy (preferred prefix)

C_6H_5-O–
phenoxy (preferred prefix)

$(CH_3)_3C$-O–
tert-butoxy (preferred prefix)
(no substitution)

The following prefix is retained for use only in general nomenclature; no substitution is allowed:

$(CH_3)_2CH$-O–
isopropoxy
1-methylethoxy
(propan-2-yl)oxy (preferred prefix)

The prefixes ‘*sec*-butoxy’ and ‘isobutoxy’ are no longer recommended:

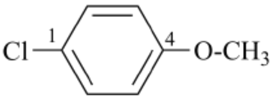
CH_3-CH_2-$CH(CH_3)$-O–
(butan-2-yl)oxy (preferred prefix)
1-methylpropoxy
(not *sec*-butoxy)

$(CH_3)_2CH$-CH_2-O–
2-methylpropoxy (preferred prefix)
(not isobutoxy)

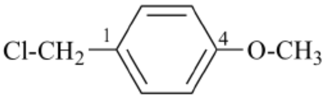
P-63.2.3 Retained names of ethers

Anisole, C_6H_5-O-CH_3, is the only name in the class of ethers which is retained both as a preferred IUPAC name and for use in general nomenclature. For preferred IUPAC names, no substitution is allowed; for general nomenclature substitution is allowed on the ring and on the side chain under certain conditions (see P-34.1.1.4).

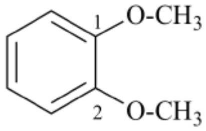
Examples:



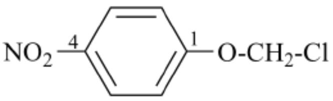
1-chloro-4-methoxybenzene (PIN;
no substitution on anisole for PINs)
4-chloroanisole



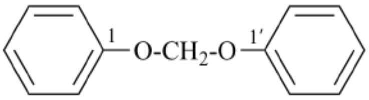
1-(chloromethyl)-4-methoxybenzene (PIN;
no substitution on anisole for PINs)
4-(chloromethyl)anisole
4-methoxybenzyl chloride
(substitution rules for benzyl see P-29.6.2.1)



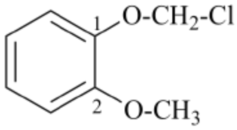
1,2-dimethoxybenzene (PIN;
no substitution on anisole for PINs)
2-methoxyanisole
(see P-34.1.1.4 and P-15.1.8.2 for substitution rules for anisole)



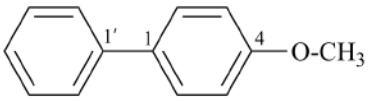
1-(chloromethoxy)-4-nitrobenzene (PIN;
no substitution on anisole for PINs)
α-chloro-4-nitroanisole
(see P-34.1.1.4 and P-15.1.8.2 for substitution rules for anisole)



1,1′-[methylenebis(oxy)]dibenzene (PIN)
α-phenoxyanisole



1-(chloromethoxy)-2-methoxybenzene (PIN;
no substitution on anisole for PINs)
α-chloro-2-methoxyanisole
[not 2-(chloromethoxy)anisole]



4-methoxy-1,1′-biphenyl (PIN)
(not 4-phenylanisole;
no substitution on anisole for PINs)
[not 1-methoxy-4-phenylbenzene;
the biphenyl ring system is senior to a single benzene ring]

P-63.2.4 Systematic names of ethers

Ethers having the general structure R-O-R′ (R=R′, or R≠R′) have the class name ‘ether’ and are named by one of the five following methods:

(1) substitutively by prefixing the name of the R′-O– group to that of the parent hydride RH;

(2) by functional class nomenclature, using the term ‘ether’ and, when the groups are different, citing the two substituent groups in alphanumerical order;

(3) by multiplicative nomenclature, when R and R′ are cyclic components;

(4) by skeletal replacement (‘a’) nomenclature;

(5) by phane nomenclature.

Functional class names based on the class name ‘oxide’ are not recommended.

P-63.2.4.1 Names of ethers, when R and R′ are both aliphatic groups or when one is cyclic, are formed by method (1), (2), or (4). Method (1) or (4) leads to preferred IUPAC names.

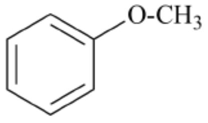
Examples:

$CH_3\text{-}O\text{-}CH_3$

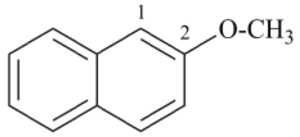
(1) methoxymethane (PIN)
(2) dimethyl ether

$CH_3\text{-}CH_2\text{-}O\text{-}CH_3$

(1) methoxyethane (PIN)
(2) ethyl methyl ether



(1) anisole (PIN; retained name)
methoxybenzene
(2) methyl phenyl ether



(1) 2-methoxynaphthalene (PIN)
(2) methyl naphthalen-2-yl ether
methyl 2-naphthyl ether

$Cl\text{-}\overset{1}{C}H_2\text{-}\overset{2}{C}H_2\text{-}O\text{-}CH_2\text{-}CH_3$

(1) 1-chloro-2-ethoxyethane (PIN)
(2) 2-chloroethyl ethyl ether
(not 2-chloroethyl ethyl oxide)

$CH_3\text{-}O\text{-}\overset{1}{C}H_2\text{-}\overset{2}{C}H_2\text{-}O\text{-}CH_3$

(1) 1,2-dimethoxyethane (PIN)
(2) ethane-1,2-diyl dimethyl ether

$CH_3\text{-}O\text{-}\overset{1}{C}H_2\text{-}\overset{2}{C}H_2\text{-}O\text{-}CH_2\text{-}CH_2\text{-}O\text{-}CH_3$

(1) 1-methoxy-2-(2-methoxyethoxy)ethane (PIN)

Skeletal replacement (‘a’) nomenclature [method (4)] generates preferred IUPAC names, when the conditions for using this type of nomenclature are met (see P-15.4); otherwise substitutive nomenclature must be used.

Example:

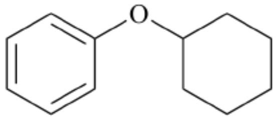
$CH_3\text{-}\overset{2}{O}\text{-}\overset{3}{C}H_2\text{-}\overset{4}{C}H_2\text{-}\overset{5}{O}\text{-}\overset{6}{C}H_2\text{-}\overset{7}{C}H_2\text{-}\overset{8}{O}\text{-}\overset{9}{C}H_2\text{-}\overset{10}{C}H_2\text{-}\overset{11}{O}\text{-}\overset{12}{C}H_3$

(4) 2,5,8,11-tetraoxadodecane (PIN)
(1) 1-methoxy-2-[2-(2-methoxyethoxy)ethoxy]ethane

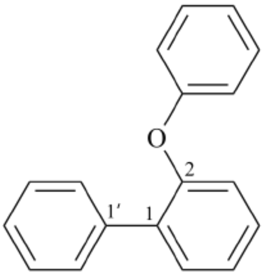
P-63.2.4.2 The names of ethers when both R and R′ groups are cyclic are formed by methods (1), (2), (3), or (5). Method (1), (3), or (5) leads to preferred IUPAC names.

When method (1), substitutive nomenclature, is used, the senior ring or ring system must be chosen as the parent hydride (see P-44).

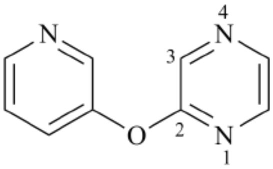
Examples:



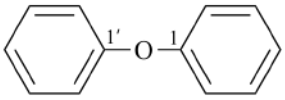
(1) (cyclohexyloxy)benzene (PIN)
(2) cyclohexyl phenyl ether



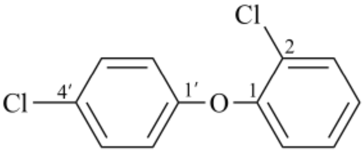
(1) 2-phenoxy-1,1′-biphenyl (PIN)
(2) biphenyl-2-yl phenyl ether



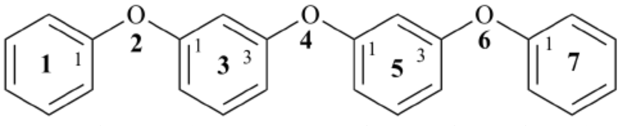
(1) 2-[(pyridin-3-yl)oxy]pyrazine (PIN)
(2) pyrazin-2-yl 3-pyridyl ether



(3) 1,1′-oxydibenzene (PIN)
(1) phenoxybenzene
(2) diphenyl ether



(1) 1-chloro-2-(4-chlorophenoxy)benzene (PIN)
(3) 2,4′-dichloro-1,1′-oxydibenzene (numbering shown)
(2) 2-chlorophenyl 4-chlorophenyl ether



(5) 2,4,6-trioxa-1,7(1),3,5(1,3)-tetrabenzenaheptaphane (PIN)
(3) 1,1′-oxybis(3-phenoxybenzene)

P-63.2.5 Names of chalcogen analogues of ethers, i.e., sulfides, selenides and tellurides

General methodology

Sulfides, R-S-R′, selenides R-Se-R′, and tellurides R-Te-R′, are named by the following methods:

(1) by prefixing the names of the substituent groups R′-S–, R′-Se–, or R′-Te–, i.e., R′-sulfanyl, R′-selanyl, and R′-tellanyl, respectively, to that of the parent hydride, RH; the prefixes ‘R′-thio’, ‘R′-seleno’ and ‘R′-telluro’ may be used in general nomenclature. The prefixes R′-sulfanyl, R′-selanyl, and R′-tellanyl are compulsory prefixes and can be attached to any atom of any parent hydride;

(2) by functional class nomenclature using the terms sulfide, selenide, and telluride for –S–, –Se–, and –Te–, respectively;

(3) by multiplicative nomenclature in the case of cyclic parent hydrides, using the prefixes sulfanediyl, –S– (not thio); selanediyl –Se– (not seleno); and tellanediyl –Te– (not telluro), respectively;

(4) by skeletal replacement (‘a’) nomenclature;

(5) by phane nomenclature;

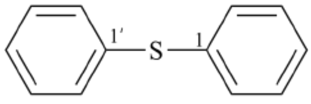
Names formed by substituting the parent hydrides oxidane, sulfane, selane, and tellane, H_2O, H_2S, H_2Se, and H_2Te, respectively, by the appropriate substituent groups are not recommended.

Names formed by functional replacement nomenclature of the retained name anisole are no longer recommended. Class names such as thiooxide are not recommended.

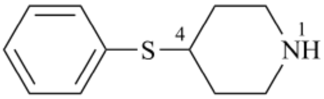
Method (1), substitutive nomenclature, gives preferred IUPAC names; method (3), (4), or (5) generates preferred IUPAC names when the conditions for their use are satisfied.

Examples:

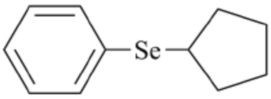
$CH_3\text{-}S\text{-}CH_3$
(1) (methylsulfanyl)methane (PIN)
(methylthio)methane
(2) dimethyl sulfide



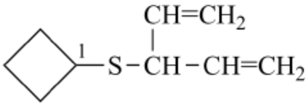
(3) 1,1′-sulfanediyldibenzene (PIN)
(not 1,1′-thiodibenzene)
(1) (phenylsulfanyl)benzene
(phenylthio)benzene
(2) diphenyl sulfide



(1) 4-(phenylsulfanyl)piperidine (PIN)
4-(phenylthio)piperidine
(2) phenyl piperidin-4-yl sulfide



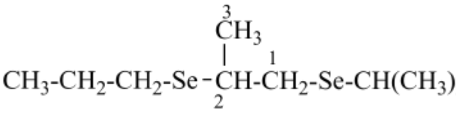
(1) (cyclopentylselanyl)benzene (PIN)
(cyclopentylseleno)benzene
(2) cyclopentyl phenyl selenide



(1) [(penta-1,4-dien-3-yl)sulfanyl]cyclobutane (PIN)
[(penta-1,4-dien-3-yl)thio]cyclobutane
(ring preferred to chain, see P-52.2.8)
(2) cyclobutyl penta-1,4-dien-3-yl sulfide
cyclobutyl 1-ethenylprop-2-en-1-yl sulfide

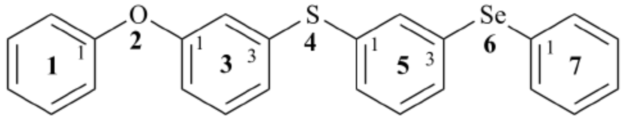
$$\overset{1}{C}H_3\text{-}\overset{2}{S}\text{-}\overset{3}{C}H_2\text{-}\overset{4}{S}\text{-}\overset{5}{C}H_2\text{-}\overset{6}{S}\text{-}\overset{7}{C}H_2\text{-}\overset{8}{C}H(CH_3)\text{-}\overset{9}{S}\text{-}\overset{10}{C}H_2\text{-}\overset{11}{S}\text{-}\overset{12}{C}H_3$$

(4) 8-methyl-2,4,6,9,11-pentathiadodecane (PIN; skeletal replacement name)
(1) 2-{[(methylsulfanyl)methyl]sulfanyl}-1-[({[(methylsulfanyl)methyl]sulfanyl}methyl)sulfanyl]propane
2-{[(methylthio)methyl]thio}-1-[({[(methylthio)methyl]thio}methyl)thio]propane
(substitutive names)

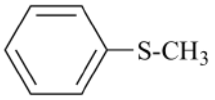


$$CH_3\text{-}CH_2\text{-}CH_2\text{-}Se\text{-}\underset{2}{\overset{\overset{3}{C}H_3}{|}{C}}H\text{-}\overset{1}{C}H_2\text{-}Se\text{-}CH(CH_3)_2$$

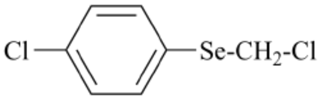
(1) 1-[(propan-2-yl)selanyl]-2-(propylselanyl)propane (PIN)
1-[(propan-2-yl)seleno]-2-(propylseleno)propane
(not 2,5-dimethyl-3,6-diselenanonane;
skeletal replacement (‘a’) nomenclature requires four heterounits, see P-51.4)



(5) 2-oxa-4-thia-6-selena-1,7(1),3,5(1,3)-tetrabenzenaheptaphane (PIN; phane name)
1-phenoxy-3-{[3-(phenylselanyl)phenyl]sulfanyl}benzene (substitutive name)
not 1-[(3-phenoxyphenyl)sulfanyl]-3-(phenylselanyl)benzene (substitutive name)
(the first substitutive name is correct because phenoxy-phenylselanyl is lower alphabetically than phenoxyphenyl-sulfanyl)



(1) (methylsulfanyl)benzene (PIN)
(not thioanisole)



(1) 1-chloro-4-[(chloromethyl)selanyl]benzene (PIN)
(not α,4-dichloroselenoanisole)

P-63.3 PEROXIDES AND CHALCOGEN ANALOGUES

P-63.3.1 Peroxides, disulfides, diselenides, and ditellurides

Compounds with the general structures R-OO-R′, R-SS-R′, R-SeSe-R′, and R-TeTe-R′ are named in the following ways:

(1) substitutively, by combining the prefix name for R′ additively with ‘peroxy’ giving the prefixes ‘R′-peroxy’ (not R′-dioxy), ‘R′-disulfanyl’, ‘R′-diselanyl’ or ‘R′-ditellanyl’ attached to the name of the parent hydride corresponding to R;

(2) by functional class nomenclature by citing the names of the groups R and R′, in alphanumerical order if two different groups are present, and the class name, peroxide, disulfide, diselenide, or ditelluride, respectively, as a separate word (class names such as dithioperoxide are not recommended);

(3) by multiplicative nomenclature, using the preferred prefixes disulfanediyl, –SS–, diselanediyl, –SeSe–, and ditellanediyl, –TeTe–, respectively; dithio, diseleno, and ditelluro may be used in general nomenclature.

(4) by skeletal replacement (‘a’) nomenclature;

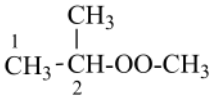
(5) by phane nomenclature.

Names formed by substituting the parent hydrides dioxidane, disulfane, diselane, and ditellane HOOH, HSSH, HSeSeH, and HTeTeH, respectively, by the appropriate substituent groups are not recommended.

Method (1), substitutive nomenclature, gives preferred IUPAC names; methods (3), (4), or (5) generate preferred IUPAC names when the conditions for their use are satisfied.

Examples:

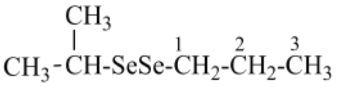
CH_3-CH_2-OO-CH_3
(1) (methylperoxy)ethane (PIN)
(2) ethyl methyl peroxide



$$\overset{1}{CH_3}\text{-}\underset{2}{\overset{\overset{3}{CH_3}}{|}}\!\!\!\!\!\!\!\!CH\text{-OO-}CH_3$$

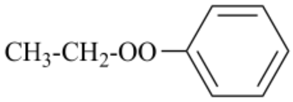
(1) 2-(methylperoxy)propane (PIN)
(2) isopropyl methyl peroxide
methyl 1-methylethyl peroxide

CH_3-SS-CH_3
(1) (methyldisulfanyl)methane (PIN)
(2) dimethyl disulfide



$$CH_3\text{-}\overset{\overset{\displaystyle CH_3}{|}}{CH}\text{-}SeSe\text{-}\overset{1}{C}H_2\text{-}\overset{2}{C}H_2\text{-}\overset{3}{C}H_3$$

(1) 1-[(propan-2-yl)diselanyl]propane (PIN)
(2) isopropyl propyl diselenide
1-methylethyl propyl diselenide



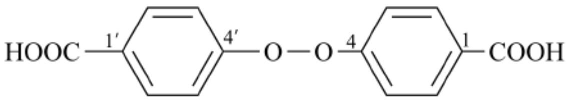
(1) (ethylperoxy)benzene (PIN)
(2) ethyl phenyl peroxide

$$CH_3\text{-}SS\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}H_2\text{-}SeSe\text{-}CH_3$$

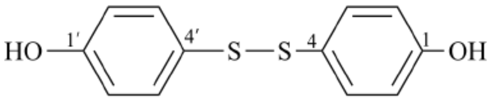
(1) 1-(methyldiselanyl)-2-(methyldisulfanyl)ethane (PIN)
1-(methyldiseleno)-2-(methyldithio)ethane

$$CH_3\text{-}SeSe\text{-}\overset{1}{Si}H_2\text{-}\overset{2}{Si}H_2\text{-}TeTe\text{-}CH_3$$

(1) 1-(methyldiselanyl)-2-(methylditellanyl)disilane (PIN)
(disilane is a preselected name, see P-12.2)
1-(methyldiseleno)-2-(methylditelluro)disilane



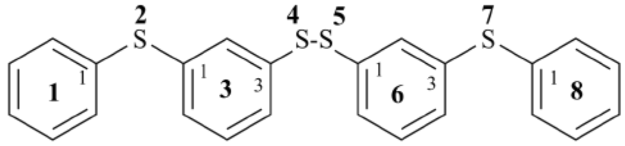
(3) 4,4′-peroxydibenzoic acid (PIN)
4-[(4-carboxyphenyl)peroxy]benzoic acid



(3) 4,4′-disulfanediyldiphenol (PIN)
4,4′-dithiodiphenol

$$\overset{1}{C}H_3\text{-}\overset{2}{S}\text{-}\overset{3}{C}H_2\text{-}\overset{4}{S}\text{-}\overset{5}{S}\text{-}\overset{6}{C}H_2\text{-}\overset{7}{C}H_2\text{-}\overset{8}{S}\text{-}\overset{9}{C}H_2\text{-}\overset{10}{C}H_2\text{-}\overset{11}{S}\text{-}\overset{12}{C}H_3$$

(4) 2,4,5,8,11-pentathiadodecane (PIN)



(5) 2,4,5,7-tetrathia-1,8(1),3,6(1,3)-tetrabenzenaoctaphane (PIN)

P-63.3.2 Mixed chalcogen analogues of peroxides

Mixed chalcogen structures such as R-XY-R′ or R-YX-R′ in which X and Y are O, S, Se, or Te atoms are named by three methods:

(1) by prefixing the names of the substituent groups R′-O–, R′-S–, R′-Se–, or R′-Te–, i.e., R′-oxy, R′-sulfanyl, R′-selanyl, and R′-tellanyl, respectively, to ‘oxy’, ‘sulfanyl’, ‘selanyl’, or ‘tellanyl’ and then to the appropriate parent hydride name. The prefixes R′-sulfanyl, R′-selanyl, and R′-tellanyl are compulsory prefixes and can be attached to any atom of any parent hydride; multiplicative nomenclature is used when the conditions for its use are fulfilled;

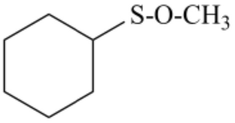
(2) by citing the prefix names of the groups R and R′, in alphanumerical order, followed by an appropriate class name ‘thioperoxide’, ‘diselenoperoxide’, ‘selenothioperoxide’, etc. Each prefix R and R′ is preceded by a capital italicized letter locant, as appropriate;

(3) by skeletal replacement (‘a’) nomenclature or phane nomenclature, when the conditions for its use are fulfilled.

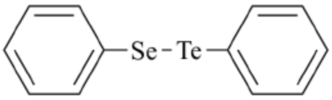
Methods (1) and (3) lead to preferred IUPAC names.

Examples:

$CH_3\text{-}CH_2\text{-}OS\text{-}CH_3$
(1) [(methylsulfanyl)oxy]ethane (PIN)
(2) *O*-ethyl *S*-methyl thioperoxide
[not ethyl methanesulfenate]



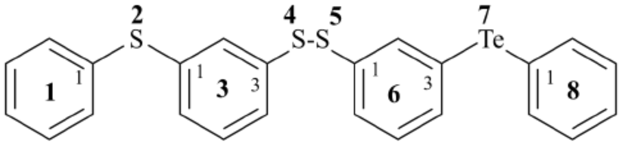
(1) (methoxysulfanyl)cyclohexane (PIN)
(2) *S*-cyclohexyl *O*-methyl thioperoxide
(not methyl cyclohexanesulfenate)



(1) [(phenylselanyl)tellanyl]benzene (PIN)
{not [(phenyltellanyl)selanyl]benzene;
phenylselan... is lower alphabetically than phenyltellan... (see P-14.5)}
(2) diphenyl selenotelluroperoxide
(not diphenyl telluroselenoperoxide;
not phenyl benzenetelluroselenate)

$$\overset{1}{C}H_3\text{-}\overset{2}{S}\text{-}\overset{3}{C}H_2\text{-}\overset{4}{S}\text{-}\overset{5}{S}\text{-}\overset{6}{C}H_2\text{-}\overset{7}{C}H_2\text{-}\overset{8}{S}\text{-}\overset{9}{C}H_2\text{-}\overset{10}{C}H_2\text{-}\overset{11}{Se}\text{-}\overset{12}{C}H_3$$

(3) 2,4,5,8-tetrathia-11-selenadodecane (PIN)
[not (methylsufanyl)methyl 2-{[2-(methylselanyl)ethyl]sulfanyl}ethanesufenothioate]



(2) 2,4,5-trithia-7-tellura-1,8(1),3,6(1,3)-tetrabenzenaoctaphane(PIN)
[not 3-(phenylsulfanyl)phenyl 3-(phenyltellanyl)benzenesulfenothioate]

P-63.4 HYDROPEROXIDES (PEROXOLS) AND CHALCOGEN ANALOGUES

P-63.4.1 Hydroperoxides

The suffix ‘peroxol’ is now introduced to name the group –OOH, formerly named by functional class nomenclature as ‘hydroperoxide’. Chalcogen analogues are names by suffixes such as ‘thioperoxol’, ‘dithioperoxol’, ‘selenoperoxol’, and ‘selenothioperoxol’.

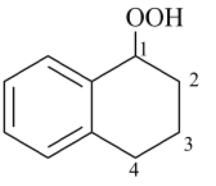
Compounds with the general structure R-OOH are called generically ‘hydroperoxides’. The class name ‘peroxols’ could be more appropriate. They are named in two ways when the –OOH group is the principal characteristic group.

(1) substitutively using the suffix ‘peroxol’;

(2) by functional class nomenclature using the class name ‘hydroperoxide’.

The prefix ‘peroxy’, not ‘dioxy’, is retained for the group –OO– (see P-63.3.1). The prefix ‘hydroperoxy’ is formed by concatenation to describe the group –OOH as a substituent in the presence of a characteristic group having priority for citation as a suffix. Method (1) leads to preferred IUPAC names.

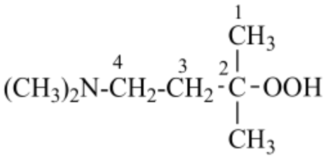
Examples:



(1) 1,2,3,4-tetrahydronaphthalene-1-peroxol (PIN)
(2) 1,2,3,4-tetrahydronaphthalen-1-yl hydroperoxide

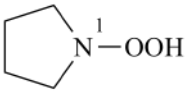
$$HOO\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}O\text{-}C_6H_5$$

2-hydroperoxy-1-phenylethan-1-one (PIN)



$$(CH_3)_2N\text{-}\overset{4}{C}H_2\text{-}\overset{3}{C}H_2\text{-}\overset{2}{C}(\overset{1}{C}H_3)(CH_3)\text{-}OOH$$

(1) 4-(dimethylamino)-2-methylbutane-2-peroxol (PIN)
(2) 4-(dimethylamino)-2-methylbutan-2-yl hydroperoxide
3-(dimethylamino)-1,1-dimethylpropyl hydroperoxide



(1) pyrrolidine-1-peroxol (PIN)
(2) pyrrolidin-1-yl hydroperoxide

P-63.4.2 Chalcogen analogues of hydroperoxides

P-63.4.2.1 Compounds having the general structure R-SOH or R-OSH are called generically ‘thioperoxols’ or ‘thiohydroperoxides’. Similarly, compounds R-SeOH or R-OSeH and R-TeOH or R-OTeH, are called ‘selenoperoxols’ or ‘selenohydroperoxides’, and ‘telluroperoxols’ or ‘tellurohydroperoxides’, respectively. When representing the principal function, they are named by two methods.

(1) by substitutive nomenclature and the appropriate suffix listed in Table 6.1 formed by functional replacement, to denote a principal function;

(2) by functional class nomenclature using the name of the class ‘thiohydroperoxide’, ‘selenohydroperoxide’ or ‘tellurohydroperoxide’. When required, the prefixes, ‘thio’, ‘seleno’ and ‘telluro’ are placed in alphabetical order, for example, ‘selenothiohydroperoxide’, etc., and the locants *O*, *S*, *Se*, or *Te* are used to designate the bonding of the R– group; when two atoms of the same element are present the class name ‘disulfide’, ‘diselenide’, or ‘ditelluride’ is used.

> Compounds of the type R-SOH, R-SeOH and R-TeOH and their chalcogen analogues were previously named sulfenic, selenenic and tellurenic acids, using the suffixes ‘sulfenic acid’, ‘selenenic acid’, and ‘tellurenic acid’, respectively.

Method (1) generates preferred IUPAC names.

Table 6.1 Suffixes denoting peroxols (hydroperoxides) modified by functional replacement nomenclature
(in decreasing order of seniority as the principal group)

–S-OH	-*SO*-thioperoxol	–Se-SH	-*SeS*-selenothioperoxol
–Se-OH	-*SeO*-selenoperoxol	–Te-SH	-*TeS*-tellurothioperoxol
–Te-OH	-*TeO*-telluroperoxol	–S-SeH	-*SSe*-selenothioperoxol
–O-SH	-*OS*-thioperoxol	–S-TeH	-*STe*-tellurothioperoxol
–O-SeH	-*OSe*-selenoperoxol	–Se-SeH	-diselenoperoxol
–O-TeH	-*OTe*-telluroperoxol	–Te-SeH	-*TeSe*-selenotelluroperoxol
–S-SH	-dithioperoxol	–Se-TeH	-*SeTe*-selenotelluroperoxol
		–Te-TeH	-ditelluroperoxol

Examples:

CH_3-SOH
(1) methane-*SO*-thioperoxol (PIN)
(2) *S*-methyl thiohydroperoxide
(no longer methanesulfenic acid)

$\overset{3}{C}H_3\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}H_2\text{-}OSH$
(1) propane-1-*OS*-thioperoxol (PIN)
(2) *O*-propyl thiohydroperoxide

CH_3-CH_2-SSH
(1) ethanedithioperoxol (PIN)
(2) ethyl hydrodisulfide
ethyl dithiohydroperoxide

CH_3-SSeH
(1) methane-*SSe*-selenothioperoxol (PIN)
(2) *S*-methyl selenothiohydroperoxide

P-63.4.2.2 Prefixes corresponding to the suffixes described in P-63.4.2.1 are obtained in two ways:

(1) by using prefixes such as ‘hydroperoxy’, –OOH; ‘disulfanyl’, –SSH, or by combining simple prefixes, ‘hydroxy’ –OH; ‘oxy-’, –O–; ‘sulfanyl’, –SH; etc.;

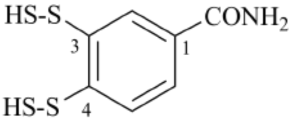
(2) by using prefixes such as dithiohydroperoxy, –SSH; *SO*-thiohydroperoxy, –OSH; *SeS*-selenothiohydroperoxy, –SSeH; etc.

Method (1) leads to preferred IUPAC names.

Examples:

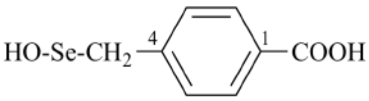
$HOO\text{-}CH_2\text{-}CH_2\text{-}OH$
2-hydroperoxyethan-1-ol (PIN)

$HSS\text{-}CH_2\text{-}COOH$
(1) disulfanylacetic acid (PIN)
(2) (dithiohydroperoxy)acetic acid



(1) 3,4-bis(disulfanyl)benzamide (PIN)
(2) 3,4-bis(dithiohydroperoxy)benzamide

$HS\text{-}O\text{-}CH_2\text{-}CH_2\text{-}CN$
(1) 3-(sulfanyloxy)propanenitrile (PIN)
(2) 3-(*SO*-thiohydroperoxy)propanenitrile



(1) 4-[(hydroxyselanyl)methyl]benzoic acid (PIN)
(2) 4-[(*OSe*-selenohydroperoxy)methyl]benzoic acid

P-63.5 CYCLIC ETHERS, SULFIDES, SELENIDES AND TELLURIDES

Cyclic ethers, sulfides, selenides and tellurides are heterocycles named by the following methods:

(1) by using preferred retained names described in P-22.2.1 (chosen first);

(2) for monocycles, by the extended Hantzsch-Widman system (see P-22.2.2) or by skeletal replacement (‘a’) nomenclature for cycles having more than ten members (see P-22.2.3);

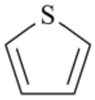
(3) by bridged fused nomenclature (see P-25.4);

(4) by using detachable prefixes ‘epoxy’, ‘epithio’, ‘episeleno’, or ‘epitelluro’ in substitutive nomenclature; these are used primarily in the nomenclature of natural products (see P-101.5.2); however they can also be used in general nomenclature.

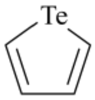
(5) by using additive names formed by the addition of the terms ‘oxide’, ‘sulfide’, ‘selenide’, or ‘telluride’ to the name of an unsaturated compound.

Names of heterocyclic compounds are preferred IUPAC names.

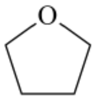
Examples:



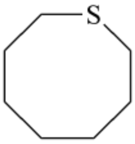
(1) thiophene (PIN)



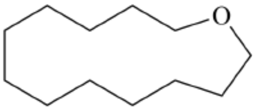
(1) tellurophene (PIN)



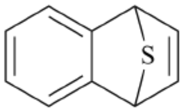
(2) oxolane (PIN)
(1) tetrahydrofuran



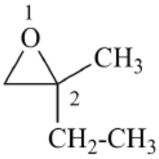
(2) thiocane (PIN)



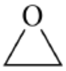
(2) oxacyclotridecane (PIN)



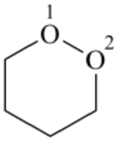
(3) 1,4-dihydro-1,4-sulfanonaphthalene (PIN)



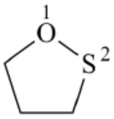
(2) 2-ethyl-2-methyloxirane (PIN)
(4) 1,2-epoxy-2-methylbutane



(2) oxirane (PIN)
(5) ethene oxide



(2) 1,2-dioxane (PIN)



(2) 1,2-oxathiolane (PIN)

P-63.6 SULFOXIDES AND SULFONES

Compounds with the general structures $R\text{-}SO\text{-}R'$ and $R\text{-}SO_2\text{-}R'$ are called generically ‘sulfoxides’ and ‘sulfones’, respectively, when R and R′ are hydrocarbyl groups. They are named in three ways as follows:

(1) substitutively, by prefixing the name of the acyl group $R'\text{-}SO\text{–}$ or $R'\text{-}SO_2\text{–}$ to the name of the parent hydride corresponding to R as described in P-65.3.2.2.2;

(2) by functional class nomenclature, using the class names ‘sulfoxide’ and ‘sulfone’, respectively;

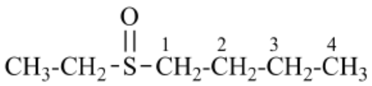
(3) by multiplicative nomenclature, except where R and R′ are alkyl groups, when the conditions for its use are satisfied.

Methods (1) and (3) generate preferred names.

Selenium and tellurium analogues are named in the same way using acyl groups derived from the appropriate seleninic, selenonic, tellurinic, and telluronic acids, and the class names ‘selenoxide’, ‘selenone’, ‘telluroxide’, ‘tellurone’. Prefixes such as ‘alkylsulfinyl’ or ‘arylsulfonyl’ may be used in general nomenclature.

Di- and polysulfones are described in P-68.4.3.2

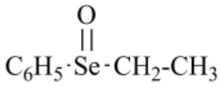
Examples:



$$CH_3\text{-}CH_2\text{-}\overset{\overset{O}{\|}}{S}\text{-}\overset{1}{C}H_2\text{-}\overset{2}{C}H_2\text{-}\overset{3}{C}H_2\text{-}\overset{4}{C}H_3$$

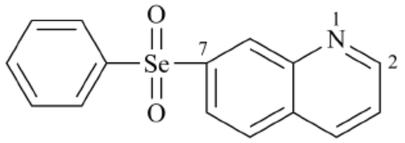
(1) 1-(ethanesulfinyl)butane (PIN)

1-(ethylsulfinyl)butane
(2) butyl ethyl sulfoxide

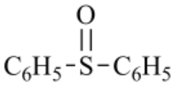


$$C_6H_5\cdot\overset{\overset{\displaystyle O}{\|}}{Se}\cdot CH_2\text{-}CH_3$$

(1) (ethaneseleninyl)benzene (PIN)
(ethylseleninyl)benzene
(2) ethyl phenyl selenoxide

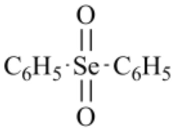


(1) 7-(benzeneselenonyl)quinoline (PIN)
7-(phenylselenonyl)quinoline
(2) phenyl quinolin-7-yl selenone
phenyl 7-quinolyl selenone



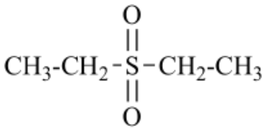
$$C_6H_5\text{-}\overset{\overset{\displaystyle O}{\|}}{S}\text{-}C_6H_5$$

(3) 1,1′-sulfinyldibenzene (PIN)
(2) diphenyl sulfoxide
(1) (benzenesulfinyl)benzene
(phenylsulfinyl)benzene



$$C_6H_5\cdot\underset{\underset{\displaystyle O}{\|}}{\overset{\overset{\displaystyle O}{\|}}{Se}}\cdot C_6H_5$$

(3) 1,1′-selenonyldibenzene (PIN)
(2) diphenyl selenone
(1) (benzeneselenonyl)benzene
(phenylselenonyl)benzene



$$CH_3\text{-}CH_2\text{-}\underset{\underset{\displaystyle O}{\|}}{\overset{\overset{\displaystyle O}{\|}}{S}}\text{-}CH_2\text{-}CH_3$$

(1) (ethanesulfonyl)ethane (PIN)
(ethylsulfonyl)ethane
(2) diethyl sulfone
Note: Multiplication of acyclic hydrocarbons is not permitted

P-63.7 POLYFUNCTIONAL COMPOUNDS

In the order of seniority of classes, hydroxy compounds and hydroperoxides are ranked in descending order after aldehydes and ketones, but before amines and imines. Chalcogen analogues are ranked after each of these classes, according to the number of O, S, Se and Te atoms. In descending order, they as follows.

(1) hydroxy compounds –OH, then their chalcogen analogues, –SH > –SeH > –TeH

(2) hydroperoxides –OOH, then their chalcogen analogues, –SOH > –SeOH > –TeOH, etc. (see Table 6.1)

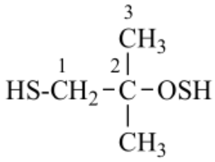
(3) amines > imines

(4) ethers, –O–, then their chalcogen analogues, –S– > –Se– > –Te–

(5) peroxides –OO–, then their chalcogen analogues, –OS– > –OSe– > –OTe–, > –SS– > –SSe– > –STe– > –SeSe– > –SeTe– > –TeTe–.

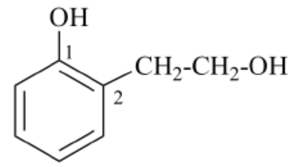
There is no seniority order between phenols and hydroxy compounds. The choice for parent hydride is decided by the maximum number of hydroxy groups cited as suffixes; and a ring is preferred to a chain when there is a choice (see P-52.2.8).

Examples:

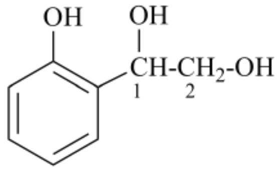


$$\mathrm{HS\text{-}\overset{1}{C}H_2\text{-}\underset{\underset{CH_3}{|}}{\overset{\overset{\overset{3}{CH_3}}{2|}}{C}}\text{-}OSH}$$

2-methyl-2-(sulfanyloxy)propane-1-thiol (PIN)



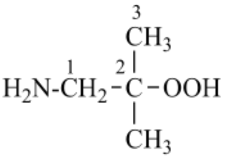
2-(2-hydroxyethyl)phenol (PIN)
2-(2-hydroxyphenyl)ethan-1-ol
(the ring is senior to the chain in the preferred name, see P-52.2.8)



1-(2-hydroxyphenyl)ethane-1,2-diol (PIN)
[not 2-(1,2-dihydroxyethyl)phenol;
two principal groups are senior to one]

$$\mathrm{HOO\text{-}\overset{1}{C}H_2\text{-}\overset{2}{C}H_2\text{-}OSeH}$$

2-(selanyloxy)ethane-1-peroxol (PIN)

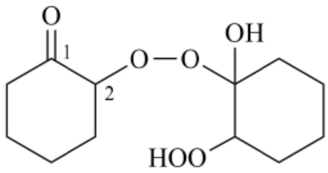


$$\mathrm{H_2N\text{-}\overset{1}{C}H_2\text{-}\underset{\underset{CH_3}{|}}{\overset{\overset{\overset{3}{CH_3}}{2|}}{C}}\text{-}OOH}$$

1-amino-2-methylpropane-2-peroxol (PIN)

$$\mathrm{CH_3\text{-}SO_2\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}H_2OH}$$

2-(methanesulfonyl)ethan-1-ol (PIN)
2-(methylsulfonyl)ethan-1-ol



2-[(2-hydroperoxy-1-hydroxycyclohexyl)peroxy]cyclohexan-1-one (PIN)
(a ketone is senior to alcohols and peroxols)

$$\mathrm{H_2N\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}H_2\text{-}OH}$$

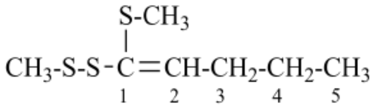
2-aminoethan-1-ol (PIN)
(not ethanolamine)

$$\mathrm{CH_3\text{-}O\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}H_2\text{-}OO\text{-}CH_2\text{-}CH_3}$$

1-(ethylperoxy)-2-methoxyethane (PIN)
(not [(2-methoxyethyl)peroxy]ethane;
the ‘PIN‘ has more substituents)

$$\mathrm{CH_3\text{-}O\text{-}\overset{1}{C}H_2\text{-}\overset{2}{C}H_2\text{-}\overset{3}{C}H_2\text{-}S\text{-}CH_3}$$

1-methoxy-3-(methylsulfanyl)propane (PIN)
1-methoxy-3-(methylthio)propane

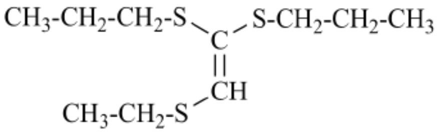


$$CH_3\text{-}S\text{-}S\text{-}\overset{\overset{\displaystyle S\text{-}CH_3}{|}}{\underset{1}{C}}{=}\underset{2}{CH}\text{-}\underset{3}{CH_2}\text{-}\underset{4}{CH_2}\text{-}\underset{5}{CH_3}$$

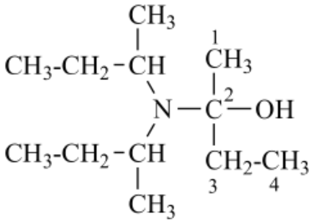
1-(methyldisulfanyl)-1-(methylsulfanyl)pent-1-ene (PIN)
{not methyl 1-(methylsulfanyl)pent-1-en-1-yl disulfide;
nor methyl[1-(methylsulfanyl)pent-1-en-1-yl]disulfane; see P-41}

$$HS\text{-}\overset{1}{C}H_2\text{-}\overset{2}{C}H_2\text{-}\overset{3}{C}H_2\text{-}Si(OCH_3)_3$$

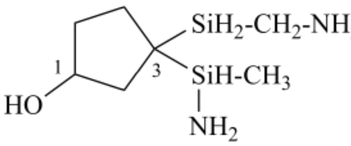
3-(trimethoxysilyl)propane-1-thiol (PIN)
[not trimethoxy(3-sulfanylpropyl)silane;
the suffix, 'thiol', has precedence over silane)



1-{[2-(ethylsulfanyl)-1-(propylsulfanyl)ethen-1-yl]sulfanyl}propane (PIN)
(multiplication of acyclic hydrocarbons is not permitted)



2-[di(butan-2-yl)amino]butan-2-ol (PIN)
2-[bis(1-methylpropyl)amino]butan-2-ol.
[not 2-(di-*sec*-butylamino)butan-2-ol]



3-[amino(methyl)silyl]-3-[(aminomethyl)silyl]cyclopentan-1-ol (PIN)
{not 3-[(aminomethyl)silyl]-3-[amino(methyl)silyl]cyclopentan-1-ol;
alphanumerical characters are identical;
at the fourth character of the name, the letter 'a' is preferred to an open parenthesis (see P-14.6)}

P-63.8 SALTS OF HYDROXY COMPOUNDS, HYDROPEROXY COMPOUNDS AND THEIR CHALCOGEN ANALOGUES

P-63.8.1 Neutral salts of hydroxy compounds and their chalcogen analogues and peroxy compounds are named by citing the cation(s) followed by the name of the anion as a separate word.

According to P-72.2.2.2.2, an anion formed by subtracting a hydron from the chalcogen atom of a hydroxy compound or a chalcogen analogue, or a peroxy compound, that can be expressed by a suffix such as 'ol', 'thiol', '-peroxol', etc., is named by using compound suffixes 'olate', 'thiolate', 'peroxolate', etc., formed by addition of the ending 'ate' to the suffixes 'ol', 'thiol', 'peroxol', etc. The multiplicative prefixes 'bis', 'tris', etc. are used before such compound suffixes, to avoid any ambiguity.

The traditional names methoxide, ethoxide, propoxide, butoxide and phenoxide, for $CH_3\text{-}O^-$, $C_2H_5\text{-}O^-$, $C_3H_7\text{-}O^-$, $C_4H_9\text{-}O^-$ and $C_6H_5\text{-}O^-$, are retained as preferred IUPAC names and aminoxide, $H_2N\text{-}O^-$, as a preselected name, and they may be substituted in the same way as the corresponding alcohols. The traditional name *tert*-butoxide for $(CH_3)_3C\text{-}O^-$ is also retained as a preferred IUPAC name but cannot be substituted. The traditional name isopropoxide for $(CH_3)_2CH\text{-}O^-$ is retained for general nomenclature but cannot be substituted.

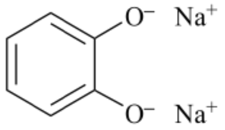
Examples:

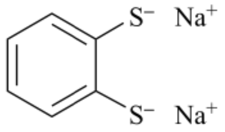
$CH_3\text{-}O^-\ Na^+$
sodium methoxide (PIN)
sodium methanolate

$CH_3\text{-}CH_2\text{-}CH_2\text{-}O^-\ Na^+$
sodium propoxide (PIN)
sodium propan-1-olate

$(CH_3)_2CH\text{-}O^-\ K^+$
potassium propan-2-olate (PIN)
potassium isopropoxide

$C_6H_5\text{-}O^-\ Li^+$
lithium phenoxide (PIN)
lithium phenolate

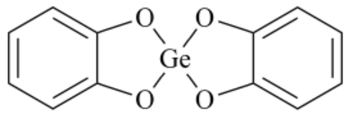

disodium benzene-1,2-bis(olate) (PIN)


disodium benzene-1,2-bis(thiolate) (PIN)

$(C_6H_5\text{-}O^-)_4\ Pb^{4+}$
lead tetraphenoxide (PIN)

P-63.8.2 Cyclic salts are named as heterocycles

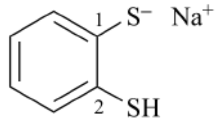
Example:


2,2′-spirobi[[1,3,2]benzodioxagermole] (PIN)

P-63.8.3 Partial salts of polyols and their chalcogen analogues are named substitutively on the basis of the corresponding anion:

Examples:

$HO\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}O^-\ Na^+$
sodium 3-hydroxypropan-1-olate (PIN)


sodium 2-sulfanylbenzene-1-thiolate (PIN)

P-64 KETONES, PSEUDOKETONES, HETERONES AND CHALCOGEN ANALOGUES

P-64.0 Introduction
P-64.1 Definitions
P-64.2 Ketones
P-64.3 Pseudoketones
P-64.4 Heterones
P-64.5 Carbonyl groups as prefixes
P-64.6 Chalcogen analogues of ketones, pseudoketones and heterones
P-64.7 Polyfunctional ketones, pseudoketones and heterones
P-64.8 Acyloins

P-64.0 INTRODUCTION

The substitutive nomenclature of ketones is well established. The suffix ‘one’ is used to denote a principal characteristic group, and the prefix ‘oxo’ is used when a characteristic group having seniority is present. The suffix ‘one’ and the prefix ‘oxo’ were indiscriminately used to name some classes of compounds other than ketones. Full systematization based on the strict application of the suffix ‘one’ for denoting the principal characteristic group =O is recommended in this Section.

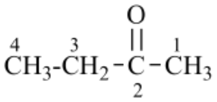
Traditionally, the nomenclature of ketones was described with that of aldehydes. In these recommendations, the two classes are discussed separately (for aldehydes, see P-66.6), to emphasize the similarities between carboxylic acids and aldehydes with respect to nomenclature. Finally, to avoid fragmentation, the nomenclature of acetals and ketals is discussed with that of aldehydes in Section P-66.6.

Rules on ketones and their chalcogen analogues, discussed as Rules C-311 to C-318 in the 1979 Recommendations (ref. 1) and Rules R-5.6.2 in the 1993 Recommendations (ref. 2) are superseded by the corresponding rules described in this Section, P-64.

P-64.1 DEFINITIONS

P-64.1.1 Ketones are defined classically as compounds in which a carbonyl group is bonded to two carbon atoms: R_2CO (neither R may be H) (see ref. 23).

Example:



$$\overset{4}{\mathrm{C}}\mathrm{H_3\text{-}}\overset{3}{\mathrm{C}}\mathrm{H_2\text{-}}\underset{2}{\overset{\overset{\mathrm{O}}{\|}}{\mathrm{C}}}\mathrm{\text{-}}\overset{1}{\mathrm{C}}\mathrm{H_3}$$

butan-2-one (PIN)

P-64.1.2 Pseudoketones and heterones

The adjunction of these two new subclasses to the general class of ketones, clarifies the general use of suffixes and prefixes in substitutive nomenclature by always giving precedence to suffixes that designate a principal characteristic group.

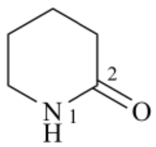
P-64.1.2.1 Pseudoketones

Pseudoketones are of two types:

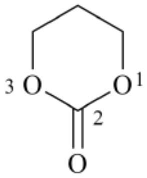
(a) cyclic compounds in which a carbonyl group in a ring is bonded to one or two skeletal heteroatoms; or

(b) compounds in which an acyclic carbonyl group is bonded to one or two acyclic skeletal heteroatoms, except nitrogen, halogen, or pseudohalogen atoms, or to a heteroatom of a ring or ring system. When the heteroatom of the ring is a nitrogen atom the compound has been called an unexpressed or 'hidden amide'.

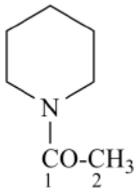
Examples:



(a) piperidin-2-one (PIN)



(a) 1,3-dioxan-2-one (PIN)



(b) 1-(piperidin-1-yl)ethan-1-one (PIN)
1-acetylpiperidine (a 'hidden amide')

$\mathrm{H_3Si\text{-}\overset{1}{C}O\text{-}\overset{2}{C}H_3}$

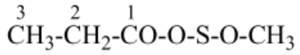
(b) 1-silylethan-1-one (PIN)
acetylsilane

$\mathrm{H_2P\text{-}\overset{1}{C}O\text{-}\overset{2}{C}H_2\text{-}\overset{3}{C}H_3}$

(b) 1-phosphanylpropan-1-one (PIN)
propanoylphosphane

$\mathrm{\overset{2}{C}H_3\text{-}\overset{1}{C}O\text{-}SS\text{-}O\text{-}CH_3}$

(b) 1-(methoxydisulfanyl)ethan-1-one (PIN)
(see also P-68.4.2)



$$\overset{3}{C}H_3\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}O\text{-}O\text{-}S\text{-}O\text{-}CH_3$$

(b) 1-[(methoxysulfanyl)oxy]propan-1-one (PIN)
(see also P-68.4.2)

P-64.1.2.2 Heterones

Heterones are compounds having an oxygen atom formally doubly bonded to a heteroatom (see P-61.6 and P-64.4; see also P-68). They are named in the same way as ketones except when expressed as compulsory prefixes, such as sulfonyl (see Table 5.1 and P-59.1.9)

Examples:

$CH_3\text{-}PO_2$
methyl-λ^5-phosphanedione (PIN)
methyldi(oxo)-λ^5-phosphane
(not phosphomethane)

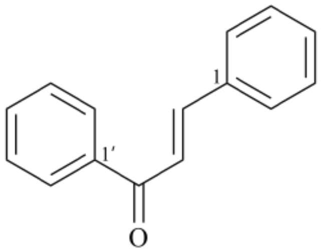
$CH_3SiH{=}O$
methylsilanone (PIN)
methyl(oxo)silane

$C_6H_5\text{-}P{=}O$
phenylphosphanone (PIN)
oxo(phenyl)phosphane
(not phosphorosobenzene)

P-64.2 KETONES

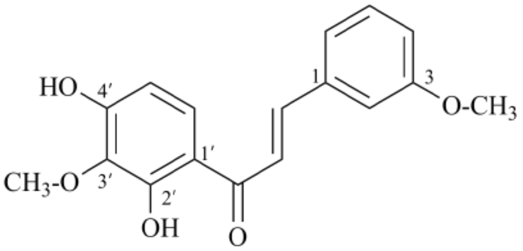
P-64.2.1 Retained names

P-64.2.1.1 The name ‘chalcone’ is the only retained name as a preferred IUPAC name and is limited to ring substitution only by characteristic groups lower than ‘ketone’. Chalcone refers only to the *trans*- or (*E*)- stereoisomer.

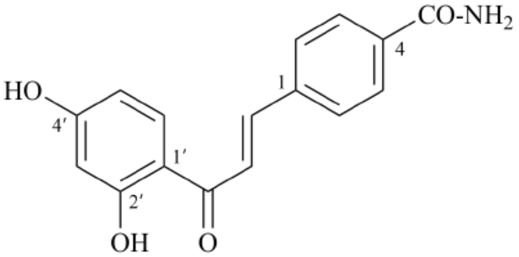


chalcone (PIN)
(2*E*)-1,3-diphenylprop-2-en-1-one

Examples:



2′,4′-dihydroxy-3,3′-dimethoxychalcone (PIN)
(2*E*)-1-(2,4-dihydroxy-3-methoxyphenyl)-3-(3-methoxyphenyl)prop-2-en-1-one

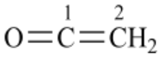


4-[(1*E*)-3-(2,4-dihydroxyphenyl)-3-oxoprop-1-en-1-yl]benzamide (PIN)
(not 2′,4′-dihydroxychalcone-4-carboxamide)

P-64.2.1.2 For use in general nomenclature, only the names acetone and 1,4-benzoquinone, together with naphthoquinone and anthraquinone with locants, are retained with substitution on the corresponding structures. The name ketene is retained, but only for general nomenclature with substitution restricted to prefixes listed in P-15.1.8.2. The names acetophenone and benzophenone are retained only for general nomenclature, but no substitution is allowed. Substitutive names, systematically constructed, are the preferred IUPAC names for ketones (see P-64.2.2)

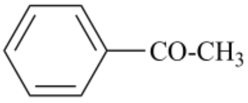
Examples:

$H_3C\text{-}CO\text{-}CH_3$
acetone
propan-2-one (PIN)

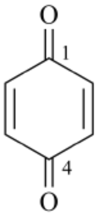


$O{=}\overset{1}{C}{=}\overset{2}{C}H_2$

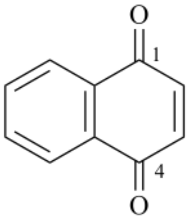
ketene
ethenone (PIN)



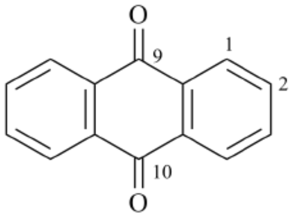
acetophenone
1-phenylethan-1-one (PIN)



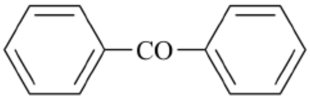
1,4-benzoquinone
cyclohexa-2,5-diene-1,4-dione (PIN)
(not benzoquinone)



1,4-naphthoquinone
(1,4 isomer shown)
naphthalene-1,4-dione (PIN)
(not naphthoquinone)

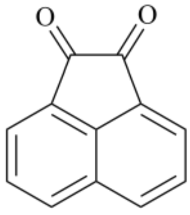


9,10-anthraquinone
anthracene-9,10-dione (PIN)
(not anthraquinone)

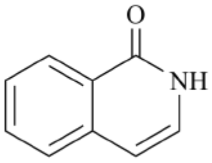


benzophenone
diphenylmethanone (PIN)
(not 1,1′-carbonyldibenzene)

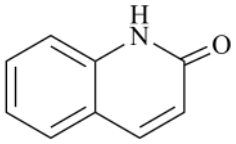
P-64.2.1.3 The following trivial names for ketones have been used in past recommendations but are no longer accepted even in general nomenclature.



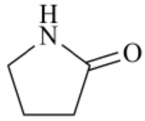
acenaphthylene-1,2-dione (PIN)
(not acenaphthoquinone)



isoquinolin-1(2*H*)-one (PIN)
[not isoquinolone (1-isomer shown)]



quinolin-2(1*H*)-one (PIN)
[not quinolone (2-isomer shown)]



pyrrolidin-2-one (PIN)
[not pyrrolidone (2-isomer shown)]

C_6H_5-CO-CO-C_6H_5
diphenylethanedione (PIN)
(not benzil)

CH_3-CO-CO-CH_3
butane-2,3-dione (PIN)
(not biacetyl)

C_6H_5-CO-CH_2-CH_3
1-phenylpropan-1-one (PIN)
(not propiophenone)

P-64.2.2 Systematic construction of names for ketones.

P-64.2.2.1 Acyclic ketones

Unsubstituted acyclic ketones are systematically named in two ways:

(1) substitutively, using the suffix ‘one’ and the prefix ‘oxo’; the presence of several ‘one’ characteristic groups is denoted by the numerical multiplying prefixes ‘di’, ‘tri’, etc.; the final letter ‘a’ of a numerical multiplying prefix is elided before the suffix ‘-one’, for example, ‘tetrone’;

(2) by functional class nomenclature using the class names ‘ketone’, ‘diketone’ etc.; substituent groups are placed, as separate words, in alphanumerical order before the class name.

Method (1) generates preferred IUPAC names.

Examples:

$\overset{1}{C}H_3\text{-}\overset{2}{C}O\text{-}\overset{3}{C}H_3$
propan-2-one (PIN)
dimethyl ketone
acetone

$\overset{4}{C}H_3\text{-}\overset{3}{C}H_2\text{-}\overset{2}{C}O\text{-}\overset{1}{C}H_3$
butan-2-one (PIN)
ethyl methyl ketone

(not methyl ethyl ketone;
groups must be cited in alphanumerical order)

$\overset{7}{C}H_3\text{-}\overset{6}{C}H_2\text{-}\overset{5}{C}H_2\text{-}\overset{4}{C}H_2\text{-}\overset{3}{C}O\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}H_3$

heptan-3-one (PIN)
butyl ethyl ketone

$\overset{25}{C}H_3\text{-}[CH_2]_5\text{-}\overset{19}{C}O\text{-}CH_2\text{-}\overset{17}{C}O\text{-}[CH_2]_7\text{-}\overset{9}{C}O\text{-}CH_2\text{-}\overset{7}{C}O\text{-}[CH_2]_5\text{-}\overset{1}{C}H_3$

pentacosane-7,9,17,19-tetrone (PIN)

$\overset{6}{C}H_3\text{-}\overset{5}{C}H(CH_3)\text{-}\overset{4}{C}H_2\text{-}\overset{3}{C}H_2\text{-}\overset{2}{C}O\text{-}\overset{1}{C}H_3$

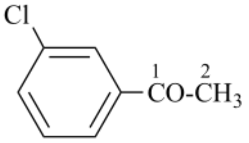
5-methylhexan-2-one (PIN)
methyl 3-methylbutyl ketone
(not isopentyl methyl ketone)

$C_6H_5\text{-}\overset{1}{C}H_2\text{-}\overset{2}{C}O\text{-}\overset{3}{C}H_3$

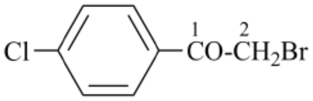
1-phenylpropan-2-one (PIN)
benzyl methyl ketone

$C_6H_5\text{-}\overset{1}{C}O\text{-}\overset{2}{C}H_3$

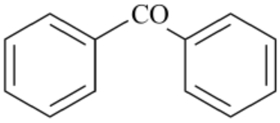
1-phenylethan-1-one (PIN)
acetophenone (no substitution)



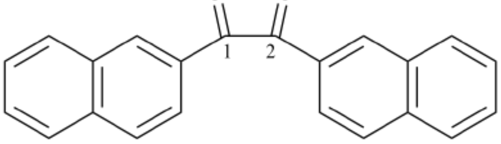
1-(3-chlorophenyl)ethan-1-one (PIN)
(not 3′-chloroacetophenone;
no substitution allowed for acetophenone)



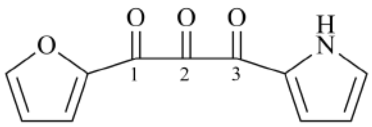
2-bromo-1-(4-chlorophenyl)ethan-1-one (PIN)
(not 4-chlorophenacyl bromide;
not 2-bromo-4′-chloroacetophenone;
no substitution allowed for acetophenone)



diphenylmethanone (PIN)
benzophenone
diphenyl ketone



di(naphthalen-2-yl)ethanedione (PIN)
di(2-naphthyl)ethanedione
di(2-naphthyl) diketone



1-(furan-2-yl)-3-(1*H*-pyrrol-2-yl)propane-1,2,3-trione (PIN)
1-(2-furyl)-3-(pyrrol-2-yl)propanetrione
2-furyl pyrrol-2-yl triketone

P-64.2.2.2 Cyclic ketones

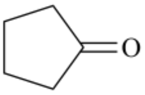
Names of cyclic ketones are formed substitutively by using the suffix ‘one’. As the formation of ketones is achieved by the conversion of a methylene, >CH_2, group into a >C=O group, the suffix ‘one’ with appropriate locants can be added to the name of parent hydrides having such groups. Methylene groups occur in saturated rings and ring systems and in mancude compounds having indicated hydrogen atoms.

Compounds not having suitably located indicated hydrogen atoms or composed only of =CH– groups, must be hydrogenated in order to create >CH_2 groups; when the hydrogenation operation occurs simultaneously with substitution by the >C=O, it is called ‘added indicated hydrogen’ (see P-14.7 and P-58.2.2). The ‘added indicated hydrogen’ method generates preferred IUPAC names.

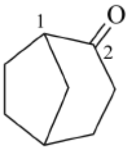
P-64.2.2.2.1 Alicyclic ketones

Ketones resulting from the substitution of >CH_2 groups are named substitutively using the suffix ‘one’ to designate the principal characteristic group.

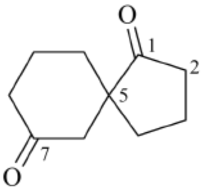
Examples:



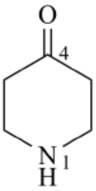
cyclopentanone (PIN)



bicyclo[3.2.1]octan-2-one (PIN)



spiro[4.5]decane-1,7-dione (PIN)

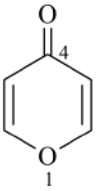


piperidin-4-one (PIN)

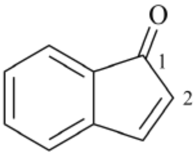
P-64.2.2.2.2 Ketones derived from mancude parent hydrides

Ketones derived from mancude parent hydrides having indicated hydrogen atoms are named by direct substitution of a >CH_2 group as indicated in P-64.2.2.2.1. When no indicated hydrogen is present, the methodology of ‘added indicated hydrogen’ is applied (see P-14.7 and P-58.2.2).

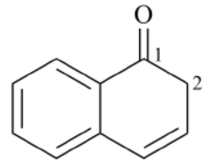
Examples:



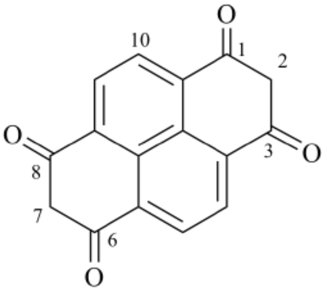
4*H*-pyran-4-one (PIN)
pyran-4-one



1*H*-inden-1-one (PIN)
inden-1-one



naphthalen-1(2*H*)-one (PIN)
1,2-dihydronaphthalen-1-one
(see P-58.2)

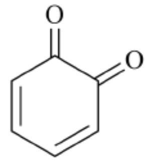


pyrene-1,3,6,8(2*H*,7*H*)-tetrone (PIN)
1,2,3,6,7,8-hexahydropyrene-1,3,6,8-tetrone
(see P-58.2)

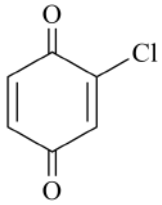
P-64.2.2.2.3 Quinones

No retained quinone names are used as preferred IUPAC names. The name 1,4-benzoquinone, and those of naphthoquinones and anthraquinones with locants, are retained for use in general nomenclature with substitution. All other quinones are named systematically using substitutive nomenclature in accordance with P-64.2.2.2.2. Diketones derived from mancude compounds without indicated hydrogen atoms by conversion of two or four =CH– groups into >C=O groups with any rearrangement of double bonds to a quinonoid structure are named systematically (see P-64.2.2.2.2).

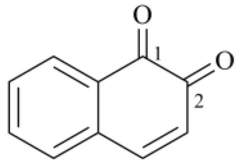
Examples:



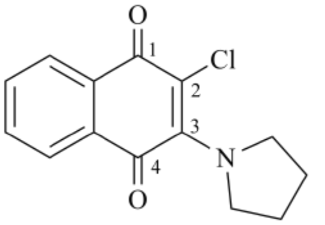
cyclohexa-3,5-diene-1,2-dione (PIN)
(not 1,2-benzoquinone)
(not *o*-benzoquinone)



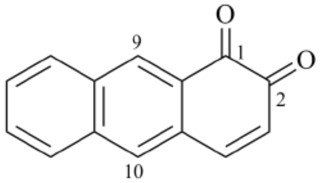
2-chlorocyclohexa-2,5-diene-1,4-dione (PIN)
2-chloro-1,4-benzoquinone
(not 2-chloro-*p*-benzoquinone)



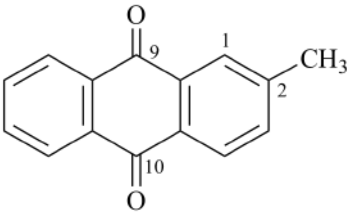
naphthalene-1,2-dione (PIN)
1,2-naphthoquinone



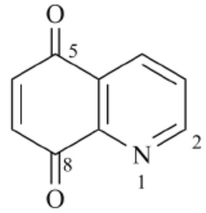
2-chloro-3-(pyrrolidin-1-yl)naphthalene-1,4-dione (PIN)
2-chloro-3-(pyrrolidin-1-yl)-1,4-naphthoquinone



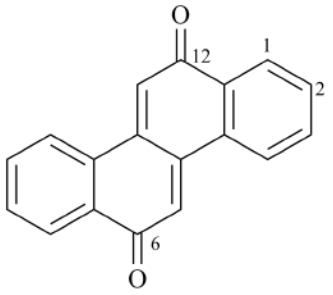
anthracene-1,2-dione (PIN)
1,2-anthraquinone



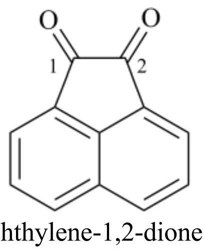
2-methylanthracene-9,10-dione (PIN)
2-methyl-9,10-anthraquinone



quinoline-5,8-dione (PIN)
(not quinoline-5,8-quinone)



chrysene-6,12-dione (PIN)
(not chrysene-6,12-quinone)

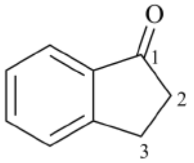


acenaphthylene-1,2-dione (PIN)
(not acenaphthoquinone)

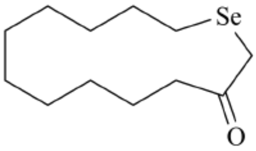
P-64.2.2.3 Seniority order for numbering

When there is a choice for numbering, the starting point and the direction of numbering of a compound are chosen so as to give lowest locants to the structural features (if present) listed in P-14.4. Rule P-52.2.8 is applied when a choice for the principal chain or senior ring system is required.

Examples:



2,3-dihydro-1*H*-inden-1-one (PIN; see P-58.2)
indan-1-one



1-selenacyclotridecan-3-one (PIN)

$\overset{1}{\mathrm{C}}\mathrm{H_3}\text{-}\overset{2}{\mathrm{Si}}\mathrm{H_2}\text{-}\mathrm{CH_2}\text{-}\overset{4}{\mathrm{Si}}\mathrm{H_2}\text{-}\mathrm{CH_2}\text{-}\overset{6}{\mathrm{Si}}\mathrm{H_2}\text{-}\mathrm{CH_2}\text{-}\overset{8}{\mathrm{Si}}\mathrm{H_2}\text{-}\mathrm{CH_2}\text{-}\overset{10}{\mathrm{C}}\mathrm{O}\text{-}\overset{11}{\mathrm{C}}\mathrm{H_3}$

2,4,6,8-tetrasilaundecan-10-one (PIN)

$\overset{4}{\mathrm{C}}\mathrm{H_2}\text{=}\overset{3}{\mathrm{C}}\mathrm{H}\text{-}\overset{2}{\mathrm{C}}\mathrm{O}\text{-}\overset{1}{\mathrm{C}}\mathrm{H_3}$

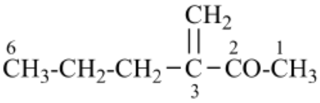
but-3-en-2-one (PIN)

$\overset{5}{\mathrm{C}}\mathrm{H_3}\text{-}\overset{4}{\mathrm{C}}\equiv\overset{3}{\mathrm{C}}\text{-}\overset{2}{\mathrm{C}}\mathrm{O}\text{-}\overset{1}{\mathrm{C}}\mathrm{H_3}$

pent-3-yn-2-one (PIN)

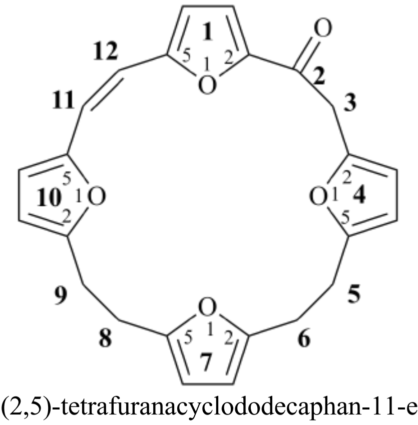
$\overset{1}{\mathrm{C}}\mathrm{H_2}\text{=}\overset{2}{\mathrm{C}}\mathrm{H}\text{-}\overset{3}{\mathrm{C}}\mathrm{O}\text{-}\overset{4}{\mathrm{C}}\equiv\overset{5}{\mathrm{C}}\mathrm{H}$

pent-1-en-4-yn-3-one (PIN)

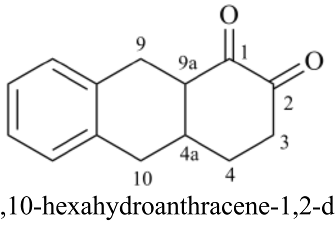


$\overset{6}{\mathrm{C}}\mathrm{H_3}\text{-}\mathrm{CH_2}\text{-}\mathrm{CH_2}-\underset{3}{\overset{\overset{\mathrm{CH_2}}{||}}{\mathrm{C}}}-\overset{2}{\mathrm{C}}\mathrm{O}\text{-}\overset{1}{\mathrm{C}}\mathrm{H_3}$

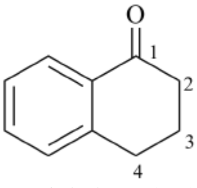
3-methylidenehexan-2-one (PIN)



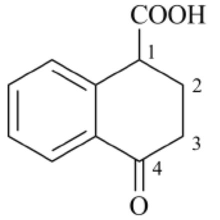
(11*Z*)-1,4,7,10(2,5)-tetrafuranacyclododecaphan-11-en-2-one (PIN)



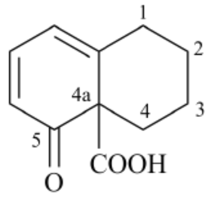
3,4,4a,9,9a,10-hexahydroanthracene-1,2-dione (PIN)
3,4,4a,9,9a,10-hexahydro-1,2-anthraquinone
1,2,3,4,4a,9,9a,10-octahydroanthracene-1,2-dione (see P-58.2)



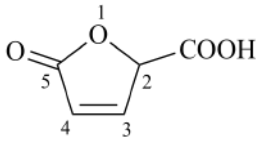
3,4-dihydronaphthalen-1(2*H*)-one (PIN)
1,2,3,4-tetrahydronaphthalen-1-one (see P-58.2)



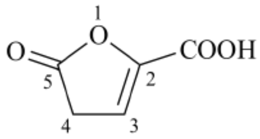
4-oxo-1,2,3,4-tetrahydronaphthalene-1-carboxylic acid (PIN)



5-oxo-1,3,4,5-tetrahydronaphthalene-4a(2*H*)-carboxylic acid (PIN)



5-oxo-2,5-dihydrofuran-2-carboxylic acid (PIN)

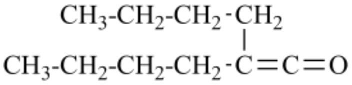


5-oxo-4,5-dihydrofuran-2-carboxylic acid (PIN)

P-64.2.2.4 Ketenes

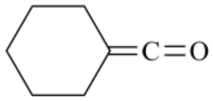
Ketene is the class name for $H_2C=C=O$ and its derivatives; the name ketene can be used in general nomenclature to name the unsubstituted structure and derivatives named by compulsory prefixes (see Table 5.1). Other derivatives are named by using the principles for naming ketones.

Examples:



$$\begin{array}{l} \qquad CH_3\text{-}CH_2\text{-}CH_2\text{-}CH_2 \\ \qquad\qquad\qquad\qquad\quad | \\ CH_3\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}C=C=O \end{array}$$

2-butylhex-1-en-1-one (PIN)
(not dibutylketene)



cyclohexylidenemethanone (PIN)

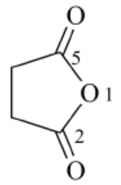
$Br_2C=C=O$
dibromoethenone (PIN)
dibromoketene

P-64.3 PSEUDOKETONES

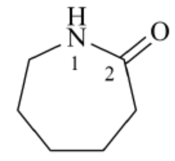
Pseudoketones are compounds having a carbonyl group joined to a carbon atom and a heteroatom, –C-CO-X–, or to two heteroatoms, –X-CO-X–, where X ≠ F, Cl, Br, I, pseudohalogen, or acyclic N. These compounds are named substitutively using the suffix 'one', in accordance with rules expressed for ketones, when required.

P-64.3.1 Cyclic anhydrides, esters and amides are named as pseudoketones; the resulting names are preferred IUPAC names.

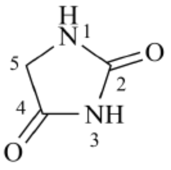
Examples:



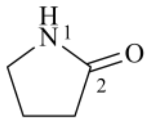
oxolane-2,5-dione (PIN)
succinic anhydride (see P-65.7.7)



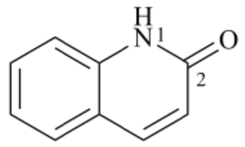
azepan-2-one (PIN)
hexano-6-lactam (see P-66.1.5.1)


H
N 1
O
5
2
4
NH
3
O

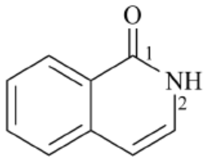
imidazolidine-2,4-dione (PIN)



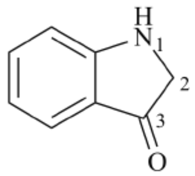
pyrrolidin-2-one (PIN)
(not 2-pyrrolidone)



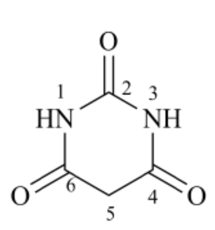
quinolin-2(1*H*)-one (PIN)
(not 1,2-dihydroquinolin-2-one)



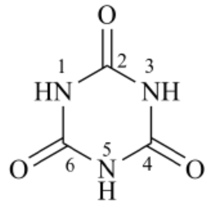
isoquinolin-1(2*H*)-one (PIN)
(not 1,2-dihydroisoquinolin-1-one)



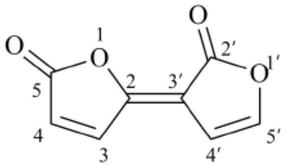
1,2-dihydro-3*H*-indol-3-one (PIN)
(not 1*H*-indol-3(2*H*)-one; see P-58.2)


O
1
2
3
HN
NH
O
6
4
O
5

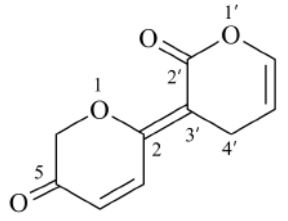
1,3-diazinane-2,4,6-trione (PIN)
pyrimidine-2,4,6(1*H*,3*H*,5*H*)-trione



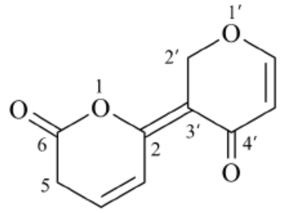
1,3,5-triazinane-2,4,6-trione (PIN)
1,3,5-triazine-2,4,6(1*H*,3*H*,5*H*)-trione



2′*H*,5*H*-[2,3′-bifuranylidene]-2′,5-dione (PIN)



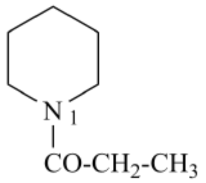
2′*H*,4′*H*-[2,3′-bipyranylidene]-2′,5(6*H*)-dione (PIN)



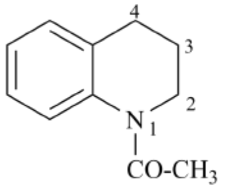
2′*H*,4′*H*-[2,3′-bipyranylidene]-4′,6(5*H*)-dione (PIN)

P-64.3.2 Acyclic pseudoketones, including those in which the carbonyl group is linked to a heteroatom of a heterocycle (hidden amides, for instance), are named substitutively by using the suffix ‘one’ to indicate the principal function. This method is preferred to that using acyl groups, when present, to denote the –CO-R group.

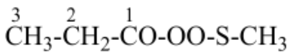
Examples:



1-(piperidin-1-yl)propan-1-one (PIN)
1-propanoylpiperidine
1-(1-oxopropyl)piperidine
(a hidden amide)

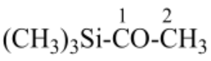


1-(3,4-dihydroquinolin-1(2*H*)-yl)ethan-1-one (PIN)
1-acetyl-1,2,3,4-tetrahydroquinoline
(a hidden amide)



$\overset{3}{C}H_3\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}O\text{-OO-S-}CH_3$

1-[(methylsulfanyl)peroxy]propan-1-one (PIN)
(see also P-68.4.2.4)



$(CH_3)_3Si\text{-}\overset{1}{C}O\text{-}\overset{2}{C}H_3$

1-(trimethylsilyl)ethan-1-one (PIN)
acetyltri(methyl)silane

P-64.4 HETERONES

Heterones are compounds having an oxygen atom formally doubly bonded to a heteroatom, see P-64.1.2.2; for heterols, see P-63.1.3; for heteroimines, see P-62.3.1.3; see also P-68.3.2.3.1 and P-68.4.3.2; and see also P-68. They are named in the same way as ketones except when they are expressed as compulsory prefixes, such as sulfonyl (see Table 5.1 and P-59.1.9).

P-64.4.1 Acyclic heterones
P-64.4.2 Thioketone and thioaldehyde oxides

P-64.4.1 Acyclic heterones are compounds having an oxygen atom doubly bonded to a heteroatom. They may be named in two ways.

(1) by the suffix 'one';

(2) by functional class names using the class name 'oxide' when the oxygen atom is bonded to a S, Se, Te, P, As, Sb, or Bi atom.

Method (1) leads to preferred IUPAC names.

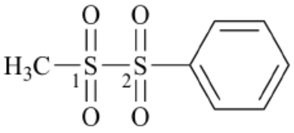
The distinction between ketones, 'C-CO-C', and aldehydes, 'C-CHO', is not retained for naming compounds having the oxygen atom linked to a heteroatom. Sulfones, sulfoxides, and related chalcogen compounds are exceptions (see P-63.6)

Examples:

HP=O
(1) phosphanone (preselected name; see P-74.2.1.4)
(2) phosphane oxide
phosphine oxide

$(CH_3)_2Si=O$
(1) dimethylsilanone (PIN)

$(C_6H_5)_3PO$
(1) triphenyl-λ^5-phosphanone (PIN, see P-74.2.1.4)
(2) triphenylphosphane oxide
triphenylphosphine oxide



(1) 1-methyl-2-phenyl-1λ^6,2λ^6-disulfane-1,1,2,2-tetrone (PIN)
(2) methyl phenyl disulfone

P-64.4.2 Thioketone and thioaldehyde oxides.

Thioketone oxides are named by three methods.

(1) substitutively, as heterones, using the λ-convention and the suffix 'one';

(2) by functional class nomenclature, using the class names 'oxide', and 'dioxide', as required.

(3) substitutively, based on the preferred parent structure

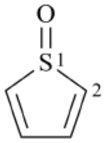
Method (1) leads to preferred IUPAC names.

Example:

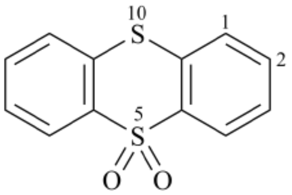
CH_3-CH_2-CH=S=O
(1) propylidene-λ^4-sulfanone (PIN)
(2) propanethial oxide
(3) 1-(oxosulfanylidene)propane

When a group –SO– or –SO_2– is part of a ring system, oxygen atom(s) are expressed substitutively by the suffix '-one' added to the name of the heterocycle in which the sulfur atoms are designated as λ^4 or λ^6 atoms (see P-14.1.3). This method generates preferred IUPAC names rather than those based on functional class nomenclature, in which the class name 'oxide' follows the name of the heterocycle, or substitutively using parent structures having nonstandard bonding chalcogen atoms.

Examples:



1*H*-1λ^4-thiophen-1-one (PIN)
thiophene oxide
1-oxo-1*H*-1λ^4-thiophene



5*H*-λ^6-thianthrene-5,5-dione (PIN)
thianthrene 5,5-dioxide
5,5-dioxo-5*H*-5λ^6-thianthrene

P-64.5 CARBONYL GROUPS AS PREFIXES

When a carbonyl group is not the principal characteristic group expressed as a suffix, it is denoted by a prefix. The traditional group ‘acetonyl’, for $CH_3\text{-}CO\text{-}CH_2\text{–}$, is retained for use in general nomenclature only; the names ‘acetonylidene’ and ‘acetonylidyne’ are not recommended even for general nomenclature. Three types of prefixes are used in the formation of preferred IUPAC names:

(1) the prefix ‘oxo’ when the doubly bonded oxygen atom (ketone, pseudoketone or heterone group) is not in position 1 of a side chain. Lowest possible locants are assigned to suffixes, and then to prefixes;

(2) carbonyl groups in position 1 of a side chain, i.e., –CO-R, are described by the appropriate acyl group name (see P-65.4 for names of acyl groups);

(3) the group –CO– is named in substitutive nomenclature as the acyl group ‘carbonyl’; the group =C=O is named in substitutive nomenclature as ‘oxomethylidene’; the substituent group –CHO is named in substitutive nomenclature as the acyl group ‘formyl’.

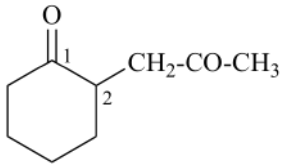
P-64.5.1 Ketones

The prefix ‘oxo’ and/or acyl prefixes are used to denote carbonyl groups when:

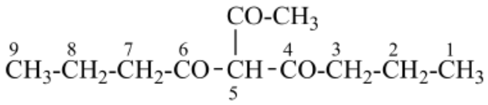
(a) all carbonyl or oxo groups cannot be cited as suffixes; or

(b) in the presence of a characteristic group having priority to be cited as suffix.

Examples:



2-(2-oxopropyl)cyclohexan-1-one (PIN)
(ring preferred to chain; see P-52.2.8)
2-acetonylcyclohexan-1-one
1-(2-oxocyclohexyl)propan-2-one

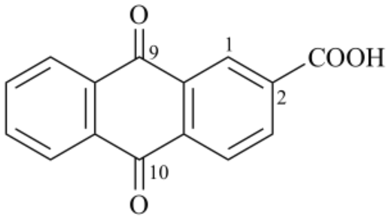


$$\overset{9}{C}H_3\text{-}\overset{8}{C}H_2\text{-}\overset{7}{C}H_2\text{-}\overset{6}{C}O\text{-}\underset{5}{\overset{\overset{\displaystyle CO\text{-}CH_3}{|}}{C}}H\text{-}\overset{4}{C}O\text{-}\overset{3}{C}H_2\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}H_3$$

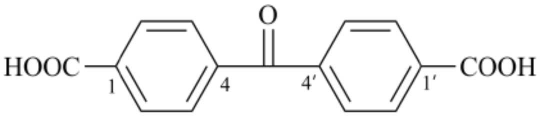
5-acetylnonane-4,6-dione (PIN)
[not 5-(1-oxoethyl)nonane-4,6-dione]

$$\overset{4}{C}H_3\text{-}\overset{3}{C}O\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}OOH$$

3-oxobutanoic acid (PIN)
(not acetylacetic acid)



9,10-dioxo-9,10-dihydroanthracene-2-carboxylic acid (PIN)
(not 9,10-anthraquinone-2-carboxylic acid)



4,4′-carbonyldibenzoic acid (PIN; multiplicative name)
4,4′-(oxomethylene)dibenzoic acid
4-(4-carboxybenzoyl)benzoic acid (substitutive name)

P-64.5.2 Pseudoketones

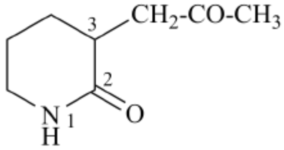
P-64.5.2.1 In cyclic pseudoketones, the prefix ‘oxo’ and/or acyl group prefixes are used to denote a carbonyl group:

(a) when all carbonyl groups cannot be cited as suffixes; or

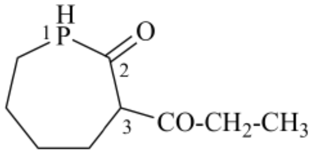
(b) in the presence of a characteristic group having priority to be cited as suffix;

Acyl prefixes are used to name pseudoketones (‘hidden amides’) having the structure R-CO-N< where the nitrogen atom is part of a ring or ring system; however, this method is recommended only for general nomenclature. Preferred IUPAC names are formed systematically (see P-64.2.2)

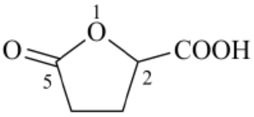
Examples:



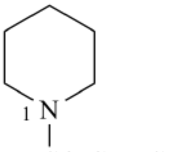
3-(2-oxopropyl)piperidin-2-one (PIN)
(ring preferred to chain, see P-52.2.8)
3-acetonylpiperidin-2-one
1-(2-oxopiperidin-3-yl)propan-2-one



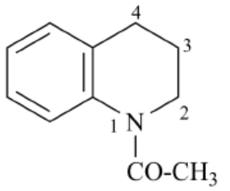
3-propanoylphosphepan-2-one (PIN)
3-propionylphosphepan-2-one



5-oxooxolane-2-carboxylic acid (PIN)



1-(piperidin-1-yl)propan-1-one (PIN)
1-propanoylpiperidine
(a ‘hidden amide’)
1-propionylpiperidine



1-(3,4-dihydroquinolin-1(2*H*)-yl)ethan-1-one (PIN)
1-acetyl-1,2,3,4-tetrahydroquinoline
(a ‘hidden amide’)

P-64.5.2.2 Acyclic pseudoketones are named in the same way; traditionally they have been named using acyl groups.

Examples:

$H_2P\text{-}CO\text{-}CH_2\text{-}CH_2\text{-}CH_3$
1-phosphanylbutan-1-one (PIN)
butanoylphosphane

$H_3Si\text{-}\overset{4}{C}O\text{-}\overset{3}{C}H_2\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}OOH$
4-oxo-4-silylbutanoic acid (PIN)
3-(silanecarbonyl)propanoic acid
3-(silylcarbonyl)propanoic acid

P-64.6 CHALCOGEN ANALOGUES OF KETONES, PSEUDOKETONES AND HETERONES

P-64.6.1 Chalcogen analogues of ketones, pseudoketones and heterones are named by using the following suffixes and prefixes:

=S ‘-thione’ and ‘sulfanylidene’ (preferred to ‘thioxo’)

=Se ‘-selone’ and ‘selanylidene’ (preferred to ‘selenoxo’)

=Te ‘-tellone’ and ‘tellanylidene’ (preferred to ‘telluroxo’)

Acyl group prefixes are named by functional replacement of O by S, Se, and Te using infixes (see P-65.1.7). The use of functional replacement prefixes ‘thio’ or ‘seleno’ with retained names is no longer recommended; all preferred IUPAC names are systematically constructed.

The use of the prefixes ‘sulfanylidene’, ‘selanylidene’ and ‘tellanylidene’, for =S, =Se, and =Te, respectively, is a change for designating of chalcogen analogs of the ‘oxo’ prefix in preferred IUPAC names. The prefixes ‘thioxo’, ‘selenoxo’, and ‘telluroxo’ derived by functional replacement nomenclature may be used in general nomenclature.

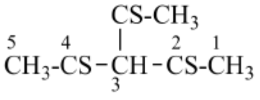
Examples:

$\overset{4}{C}H_3\text{-}\overset{3}{C}H_2\text{-}\overset{2}{C}S\text{-}\overset{1}{C}H_3$
butane-2-thione (PIN)

$\overset{1}{C}H_3\text{-}\overset{2}{C}H_2\text{-}\overset{3}{C}Se\text{-}\overset{4}{C}H_2\text{-}\overset{5}{C}H_2\text{-}\overset{6}{C}H_3$
hexane-3-selone (PIN)

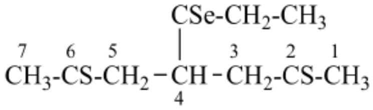
$\overset{5}{C}H_3\text{-}\overset{4}{C}S\text{-}\overset{3}{C}H_2\text{-}\overset{2}{C}S\text{-}\overset{1}{C}H_3$
pentane-2,4-dithione (PIN)

$\overset{3}{C}H_3\text{-}\overset{2}{C}S\text{-}\overset{1}{C}H_3$
propane-2-thione (PIN)
(not thioacetone)



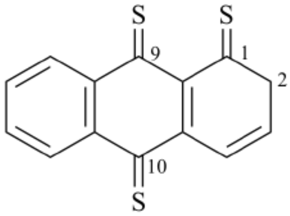
$\overset{5}{C}H_3\text{-}\overset{4}{C}S\text{-}\underset{3}{\overset{\overset{\displaystyle CS\text{-}CH_3}{|}}{C}}H\text{-}\overset{2}{C}S\text{-}\overset{1}{C}H_3$

3-(ethanethioyl)pentane-2,4-dithione (PIN)
3-(thioacetyl)pentane-2,4-dithione
3-(1-sulfanylideneethyl)pentane-2,4-dithione

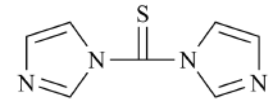


$$\overset{7}{\mathrm{CH_3}}\text{-}\overset{6}{\mathrm{CS}}\text{-}\overset{5}{\mathrm{CH_2}}-\underset{4}{\overset{\overset{\mathrm{CSe\text{-}CH_2\text{-}CH_3}}{|}}{\mathrm{CH}}}-\overset{3}{\mathrm{CH_2}}\text{-}\overset{2}{\mathrm{CS}}\text{-}\overset{1}{\mathrm{CH_3}}$$

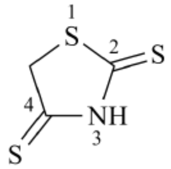
4-(propaneselenoyl)heptane-2,6-dithione (PIN)
4-(1-selanylidenepropyl)heptane-2,6-dithione



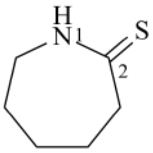
anthracene-1,9,10(2*H*)-trithione (PIN)



di(1*H*-imidazol-1-yl)methanethione (PIN)



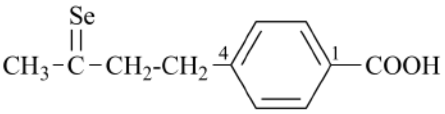
1,3-thiazolidine-2,4-dithione (PIN)



azepane-2-thione (PIN)

$$\overset{4}{\mathrm{CH_3}}\text{-}\overset{3}{\mathrm{CS}}\text{-}\overset{2}{\mathrm{CH_2}}\text{-}\overset{1}{\mathrm{COOH}}$$

3-sulfanylidenebutanoic acid (PIN)
3-thioxobutanoic acid



4-(3-selanylidenebutyl)benzoic acid (PIN)
4-(3-selenoxobutyl)benzoic acid

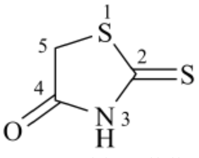
P-64.6.2 Seniority order of suffixes

The order of seniority of ketonic suffixes is C=O > C=S > C=Se > C=Te. Lowest locants are assigned in accordance with that order.

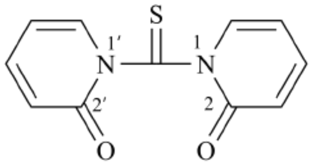
Examples:

$$\overset{5}{\mathrm{CH_3}}\text{-}\overset{4}{\mathrm{CS}}\text{-}\overset{3}{\mathrm{CH_2}}\text{-}\overset{2}{\mathrm{CO}}\text{-}\overset{1}{\mathrm{CH_3}}$$

4-sulfanylidenepentan-2-one (PIN)
4-thioxopentan-2-one



2-sulfanylidene-1,3-thiazolidin-4-one (PIN)
2-thioxo-1,3-thiazolidin-4-one

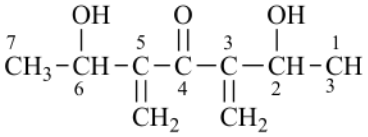


1,1′-carbonothioyldi(pyridin-2(1*H*)-one) (PIN)
1,1′-thiocarbonyldi(pyridin-2(1*H*)-one)

P-64.7 POLYFUNCTIONAL KETONES, PSEUDOKETONES AND HETERONES

P-64.7.1 Ketones, pseudoketones and heterones, and their chalcogen analogues in the order =O > =S > =Se > =Te, are senior to hydroxy compounds and their chalcogen analogues, amines, and imines in the seniority order of classes. In the presence of a characteristic group having priority to be cited as suffix as described in P-64.5 and P-64.6, they are cited as prefixes (see P-41).

Examples:

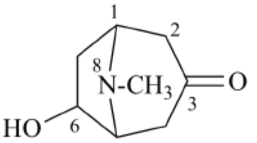


$$\overset{7}{CH_3}-\underset{6}{\overset{\overset{OH}{|}}{CH}}-\underset{\underset{CH_2}{||}}{\overset{5}{C}}-\underset{4}{\overset{\overset{O}{||}}{C}}-\underset{\underset{CH_2}{||}}{\overset{3}{C}}-\underset{2}{\overset{\overset{OH}{|}}{CH}}-\underset{3}{\overset{1}{CH}}$$

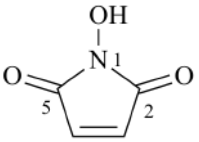
2,6-dihydroxy-3,5-dimethylideneheptan-4-one (PIN)

$$\overset{4}{CH_3}\text{-}\overset{3}{CO}\text{-}\overset{2}{CH_2}\text{-}\overset{1}{COOH}$$

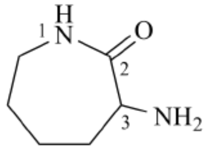
3-oxobutanoic acid (PIN)



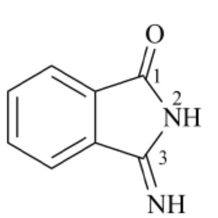
6-hydroxy-8-methyl-8-azabicyclo[3.2.1]octan-3-one
6-hydroxy-8-methyltropan-3-one



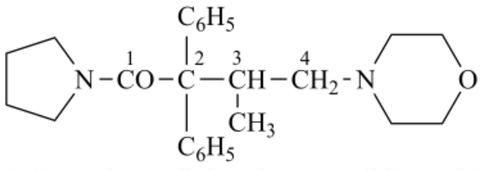
1-hydroxy-1*H*-pyrrole-2,5-dione (PIN)



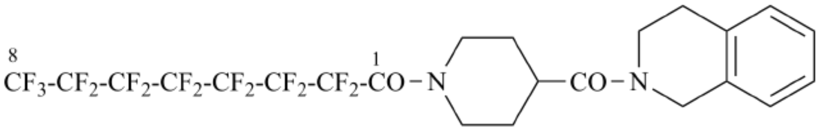
3-aminoazepan-2-one (PIN)



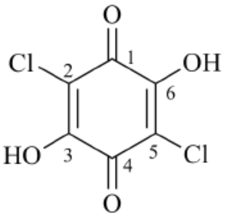
3-imino-2,3-dihydro-1*H*-isoindol-1-one (PIN)



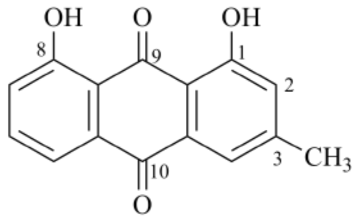
3-methyl-4-(morpholin-4-yl)-2,2-diphenyl-1-(pyrrolidin-1-yl)butan-1-one (PIN)



1-[4-(3,4-dihydroisoquinoline-2(1*H*)-carbonyl)piperidin-1-yl]-2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-pentadecafluorooctan-1-one
(PIN, the locants for the fluoro substituents are required, see P-14.3.4.5)



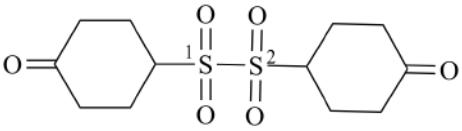
2,5-dichloro-3,6-dihydroxycyclohexa-2,5-diene-1,4-dione (PIN)
2,5-dichloro-3,6-dihydroxy-1,4-benzoquinone



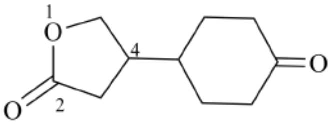
1,8-dihydroxy-3-methylanthracene-9,10-dione (PIN)
1,8-dihydroxy-3-methyl-9,10-anthraquinone

P-64.7.2 There is no seniority order difference between ketones and pseudoketones. When necessary, the maximum number of carbonyl groups or doubly bonded oxygen atoms, the seniority order between chains and rings, and between rings and ring systems, are considered, as appropriate.

Examples:



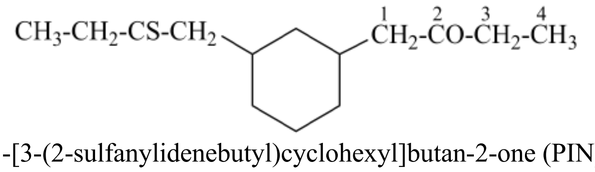
1,2-bis(4-oxocyclohexyl)-1λ^6,2λ^6-disulfane-1,1,2,2-tetrone (PIN)
[the heterone with four doubly bonded oxygen atoms is senior to cyclohexanone,
which has only one carbonyl group (see P-44.1.1)]



4-(4-oxocyclohexyl)oxolan-2-one (PIN)
[not 4-(2-oxooxolan-4-yl)cyclohexanone;
a heterocyclic ring is senior to a carbocyclic ring, see P-44.2.1)

P-64.7.3 When an oxygen atom of a ketone, pseudoketone, or heterone is replaced by a sulfur, selenium or tellurium atom, the seniority order for expression as the suffix is O > S > Se > Te.

Example:

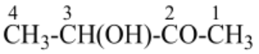


1-[3-(2-sulfanylidenebutyl)cyclohexyl]butan-2-one (PIN)
1-[3-(2-thioxobutyl)cyclohexyl]butan-2-one

P-64.8 ACYLOINS

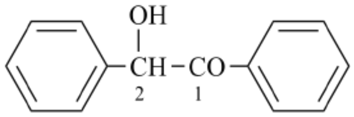
α-Hydroxy ketones, RCH(OH)-CO-R, in which R is an alkyl, aryl, or a heterocyclic group, have the class name ‘acyloins’ and are named by substitutive nomenclature as substituted ketones, in accordance with the seniority order: ketones > hydroxy compounds (see P-41). Names ending in ‘oin’ are not recommended.

Examples:

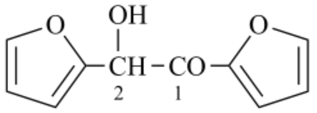


$\overset{4}{C}H_3\text{-}\overset{3}{C}H(OH)\text{-}\overset{2}{C}O\text{-}\overset{1}{C}H_3$

3-hydroxybutan-2-one (PIN)
(not acetoin)



2-hydroxy-1,2-diphenylethan-1-one (PIN)



1,2-di(furan-2-yl)-2-hydroxyethan-1-one (PIN)
1,2-di(2-furyl)-2-hydroxyethan-1-one

P-65 ACIDS, ACYL HALIDES AND PSEUDOHALIDES, SALTS, ESTERS, AND ANHYDRIDES

P-65.0 Introduction
P-65.1 Carboxylic acids and functional replacement analogues
P-65.2 Carbonic, cyanic, and di- and polycarbonic acids
P-65.3 Sulfur, selenium, and tellurium acids with chalcogen atoms directly linked to a parent hydride
P-65.4 Acyl groups as substituent groups
P-65.5 Acyl halides and pseudohalides
P-65.6 Salts and esters
P-65.7 Anhydrides and their analogues

P-65.0 INTRODUCTION

This Chapter includes acids named substitutively by means of suffixes, that is, carboxylic acids, sulfonic, sulfinic, and analogous selenium and tellurium acids. Their derivatives, such as esters, acyl halides, and anhydrides, are also included. Salts are included in this Section although anions are formally treated in Chapter P-7. Carbon acids not named substitutively, i.e., carbonic acid, cyanic acid, and the di- and polynuclear carbon acids are also included here. Mononuclear and polynuclear inorganic (noncarbon) acids used as parent structures for organic derivatives are discussed in Section P-67.

The hydrogen atom of an acid group is not substitutable for the purposes of substitutive nomenclature; replacement of acid hydrogen atoms by specific atoms or groups is called ‘functionalization’, as other classes are generated, for example esters. Substitution takes place when other hydrogen atoms in the structure are exchanged with other atoms or groups, as illustrated by the name ‘chloroacetic acid’.

P-65.1 CARBOXYLIC ACIDS AND FUNCTIONAL REPLACEMENT ANALOGUES

Carboxylic acids have the structure R-C(=O)-OH, where R can be a hydrogen atom. Nitrogenous analogues are carboxylic acids in which =O has been replaced by =NH, $=NNH_2$, =N-OH, or in which –OH has been replaced by –NH-OH. Chalcogen analogues are carboxylic acids in which one or two oxygen atoms have been replaced by sulfur, selenium, or tellurium atoms.

Names of α-amino acids, as well as carboxylic acids derived from carbohydrates, are not covered extensively in this Chapter. Traditional names are maintained, as recommended in specialized publications (refs. 18, 27), and listed in Chapter P-10 devoted to natural products.

P-65.1.1 Retained names
P-65.1.2 Systematic names
P-65.1.3 Carboximidic, carbohydrazonic, carbohydroximic, and carbohydroxamic acids
P-65.1.4 Peroxycarboxylic acids
P-65.1.5 Chalcogen analogues of carboxylic acids
P-65.1.6 Amic, anilic, and aldehydic acids
P-65.1.7 Acyl groups derived from carboxylic and related acids
P-65.1.8 Formic acid

P-65.1.1 Retained names

Carboxylic acids derived from natural sources were often given trivial names reminiscent of their animal or vegetable origin. In both 1979 and 1993, the list of these trivial names was significantly reduced, systematic names being recommended.

P-65.1.1.1 Retained names as preferred IUPAC names

Only the following five carboxylic acids retained names and are also preferred IUPAC names. All can be functionalized, but only acetic acid, benzoic acid, and oxamic acid can be substituted according to P-15.1.8.2.1; for substitution rules regarding formic acid, see P-65.1.8. Systematic substitutive names are used to generate acids modified by functional replacement.

$HCOOH$
formic acid (PIN)
methanoic acid

$HOOC\text{-}COOH$
oxalic acid (PIN)
ethanedioic acid

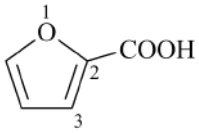
$CH_3\text{-}COOH$
acetic acid (PIN)
ethanoic acid

$C_6H_5\text{-}COOH$
benzoic acid (PIN)
benzenecarboxylic acid

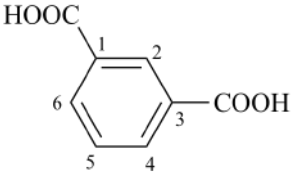
$H_2N\text{-}CO\text{-}COOH$
oxamic acid (PIN)
amino(oxo)acetic acid

P-65.1.1.2 Retained names only for general nomenclature

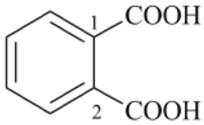
P-65.1.1.2.1 The following names are retained, but only for general nomenclature, with substitution according to P-15.1.8.2.1 allowed (see also P-34).



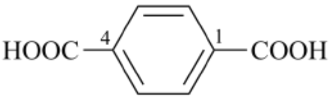
2-furoic acid (also 3-isomer)
furan-2-carboxylic acid (PIN)



isophthalic acid
benzene-1,3-dicarboxylic acid (PIN)



phthalic acid
benzene-1,2-dicarboxylic acid (PIN)



terephthalic acid
benzene-1,4-dicarboxylic acid (PIN)

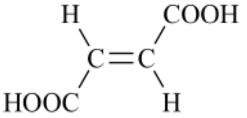
P-65.1.1.2.2 The following names are retained for general nomenclature with functionalization but no substitution is allowed. Functionalization leads to anhydrides, salts, and esters, for example, the formation of esters leads to names such as methyl butyrate.

$CH_2{=}CH\text{-}COOH$
acrylic acid
prop-2-enoic acid (PIN)

$HOOC-[CH_2]_4-COOH$
adipic acid
hexanedioic acid (PIN)

$CH_3-CH_2-CH_2-COOH$
butyric acid
butanoic acid (PIN)

$C_6H_5-CH=CH-COOH$
cinnamic acid (‘*E*’ configuration implied)
3-phenylprop-2-enoic acid (PIN;
‘*E*’ and ‘*Z*‘ isomers)

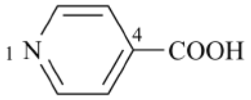

H
COOH
C=C
HOOC
H

fumaric acid
(2*E*)-but-2-enedioic acid (PIN)

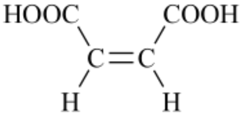
$HOOC-[CH_2]_3-COOH$
glutaric acid
pentanedioic acid (PIN)

$HOOC-CH_2-COOH$
malonic acid
propanedioic acid (PIN)

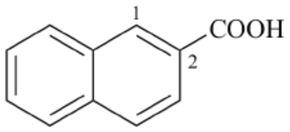
$CH_2=C(CH_3)-COOH$
methacrylic acid
2-methylprop-2-enoic acid (PIN)



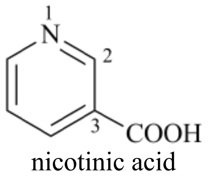
isonicotinic acid
pyridine-4-carboxylic acid (PIN)


HOOC
COOH
C=C
H
H

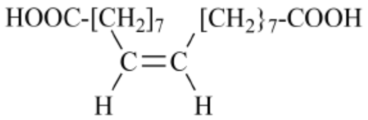
maleic acid
(2*Z*)-but-2-enedioic acid (PIN)



2-naphthoic acid (also 1-isomer)
naphthalene-2-carboxylic acid (PIN)



nicotinic acid
pyridine-3-carboxylic acid (PIN)


HOOC-[CH2]7
[CH2}7-COOH
C=C
H
H

oleic acid
(9*Z*)-octadec-9-enoic acid (PIN)

$CH_3-[CH_2]_{14}-COOH$
palmitic acid
hexadecanoic acid (PIN)

$CH_3\text{-}CH_2\text{-}COOH$
propionic acid
propanoic acid (PIN)

$CH_3\text{-}[CH_2]_{16}\text{-}COOH$
stearic acid
octadecanoic acid (PIN)

$HOOC\text{-}CH_2\text{-}CH_2\text{-}COOH$
succinic acid
butanedioic acid (PIN)

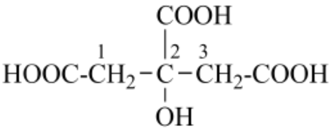
$CH_3\text{-}CO\text{-}OOH$
peracetic acid
ethaneperoxoic acid (PIN)

$C_6H_5\text{-}CO\text{-}OOH$
perbenzoic acid
benzenecarboperoxoic acid (PIN)

$H\text{-}CO\text{-}OOH$
performic acid
methaneperoxoic acid (PIN; see P-65.1.4.1)

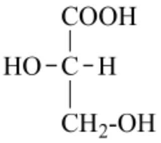
$(HOOC\text{-}CH)_2N\text{-}CH_2\text{-}CH_2\text{-}N(CH_2\text{-}COOH)_2$
ethylenediaminetetraacetic acid
N,*N*′-(ethane-1,2-diyl)bis[*N*-(carboxymethyl)glycine]
2,2′,2″,2‴-(ethane-1,2-diyldinitrilo)tetraacetic acid

P-65.1.1.2.3 The names citric acid, lactic acid, glyceric acid, pyruvic acid, and tartaric acid, related to natural products, are also retained; no substitution is recommended, but the formation of salts and esters is allowed.



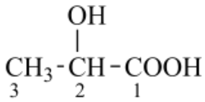
$$\mathrm{HOOC\text{-}\overset{1}{C}H_2-\overset{COOH}{\underset{OH}{\overset{2}{C}}}-\overset{3}{C}H_2\text{-}COOH}$$

citric acid
2-hydroxypropane-1,2,3-tricarboxylic acid (PIN)



$$\mathrm{HO-\overset{COOH}{\underset{CH_2\text{-}OH}{C}}-H}$$

glyceric acid
2,3-dihydroxypropanoic acid (PIN)



$$\mathrm{\underset{3}{CH_3}\text{-}\underset{2}{\overset{OH}{CH}}-\underset{1}{COOH}}$$

lactic acid
2-hydroxypropanoic acid (PIN)

$CH_3\text{-}CO\text{-}COOH$
pyruvic acid
2-oxopropanoic acid (PIN)

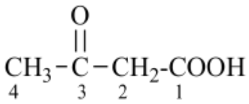
$HOOC\text{-}[CH(OH)]_2\text{-}COOH$
tartaric acid
2,3-dihydroxybutanedioic acid (PIN)
(to denote configuration, see P-102.5.6.6.5)

Names of α-amino acids related to peptides and proteins are also retained (see P-103). Some names, for example 'glycine' for $H_2N\text{-}CH_2\text{-}COOH$, are used to form systematic substitutive names (see P-103.2). Names of carboxylic acids derived from retained names of carbohydrates are also used as systematic sustitutive names (see P-102.5.6.6).

P-65.1.1.2.4 The following trivial names are no longer recommended.

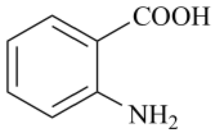
$HC\equiv C\text{-}COOH$
prop-2-ynoic acid (PIN)
(not propiolic acid)

$(CH_3)_2CH\text{-}COOH$
2-methylpropanoic acid (PIN
(not isobutyric acid)



$\underset{4}{CH_3}-\underset{3}{\overset{\overset{O}{||}}{C}}-\underset{2}{CH_2}\text{-}\underset{1}{C}OOH$

3-oxobutanoic acid (PIN)
(not acetoacetic acid)



2-aminobenzoic acid (PIN)
[not anthranilic acid (1,2-isomer only)]

$(C_6H_5)_2C(OH)\text{-}COOH$
hydroxydi(phenyl)acetic acid (PIN)
(not benzilic acid)

$HO\text{-}CH_2\text{-}COOH$
hydroxyacetic acid (PIN)
(not glycolic acid)

$OHC\text{-}COOH$
oxoacetic acid (PIN)
(not glyoxylic acid)

P-65.1.2 Systematic names

Carboxylic acids are named substitutively using the suffix ‘oic acid’ or ‘carboxylic acid’ and the prefix ‘carboxy’ to describe chain are named by replacing the final ‘e’ of the name of the corresponding hydrocarbon by the suffix ‘oic acid’. No locants are necessary to denote the positions of the carboxylic acid groups in a hydrocarbon chain; locants are used when hydrocarbon chains are modified by skeletal replacement, as shown in P-15.4.3.2.3. Except for formic acid, acetic acid, oxalic acid (see P-65.1.1.1), and oxamic acid (see P-65.1.1.1), systematically formed names are preferred IUPAC names; the names given in P-65.1.1.2 are retained names for use in general nomenclature.

Examples:

$\overset{4}{C}H_3\text{-}\overset{3}{C}H_2\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}OOH$
butanoic acid (PIN)
butyric acid

$\overset{10}{C}H_3\text{-}[CH_2]_8\text{-}\overset{1}{C}OOH$
decanoic acid (PIN)

$HOO\overset{12}{C}\text{-}[CH_2]_{10}\text{-}\overset{1}{C}OOH$
dodecanedioic acid (PIN)

$\overset{15}{C}H_3\text{-}CH_2\text{-}CH_2\text{-}\overset{12}{O}\text{-}CH_2\text{-}CH_2\text{-}\overset{9}{O}\text{-}CH_2\text{-}CH_2\text{-}\overset{6}{O}\text{-}CH_2\text{-}CH_2\text{-}\overset{3}{O}\text{-}CH_2\text{-}\overset{1}{C}OOH$
3,6,9,12-tetraoxapentadecan-1-oic acid (PIN)

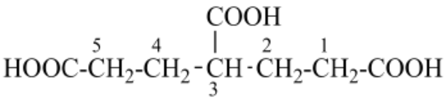
$HOO\overset{15}{C}\text{-}CH_2\text{-}CH_2\text{-}\overset{12}{O}\text{-}CH_2\text{-}CH_2\text{-}\overset{9}{O}\text{-}CH_2\text{-}CH_2\text{-}\overset{6}{O}\text{-}CH_2\text{-}CH_2\text{-}\overset{3}{O}\text{-}CH_2\text{-}\overset{1}{C}H_3$
3,6,9,12-tetraoxapentadecan-15-oic acid (PIN)

$HOO\overset{15}{C}\text{-}CH_2\text{-}\overset{12}{S}\text{-}CH_2\text{-}CH_2\text{-}\overset{10}{S}\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}\overset{6}{S}\text{-}CH_2\text{-}CH_2\text{-}\overset{3}{S}\text{-}CH_2\text{-}\overset{1}{C}OOH$
3,6,10,13-tetrathiapentadecane-1,15-dioic acid (PIN)

P-65.1.2.2 The suffix ‘carboxylic acid’ is used for all carboxylic acids not covered by P-65.1.2.1, except for benzoic acid, a retained name (see P-65.1.1.1). The carboxy group can be attached to any atom, carbon or heteroatom, of any parent hydride; the proper methodology must be applied in the case of mancude parent hydrides as exemplified in P-65.1.2.3.

P-65.1.2.2.1 If an unbranched chain is linked to more than two carboxy groups, all carboxy groups are named from the parent hydride by substitutive use of the suffix ‘carboxylic acid’, preceded by the appropriate numerical prefix ‘tri’, ‘tetra’ etc. and appropriate locants.

Examples:



$$HOOC\text{-}\overset{5}{C}H_2\text{-}\overset{4}{C}H_2\text{-}\underset{3}{\overset{\overset{COOH}{|}}{C}}H\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}H_2\text{-}COOH$$

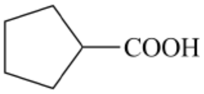
pentane-1,3,5-tricarboxylic acid (PIN)

$(HOOC)_2\overset{1}{C}H\text{-}\overset{2}{C}H(COOH)_2$

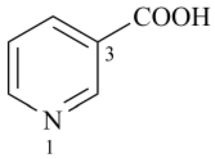
ethane-1,1,2,2-tetracarboxylic acid (PIN)

P-65.1.2.2.2 Carboxy groups attached to cyclic parent hydrides or heteroacyclic parent hydrides are always named by using the suffix ‘carboxylic acid’.

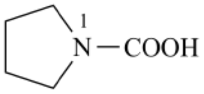
Examples:



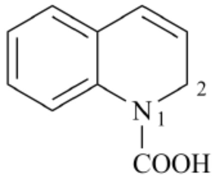
cyclopentanecarboxylic acid (PIN)



pyridine-3-carboxylic acid (PIN)
nicotinic acid



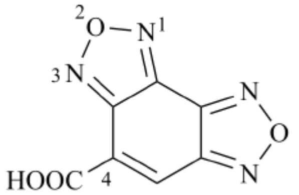
pyrrolidine-1-carboxylic acid (PIN)



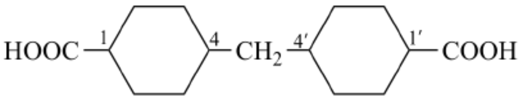
quinoline-1(2*H*)-carboxylic acid (PIN)

$H_3Si\text{-}O\text{-}SiH_2\text{-}COOH$
disiloxanecarboxylic acid (PIN)

$H_2N\text{-}NH\text{-}COOH$
hydrazinecarboxylic acid (PIN)
carbonohydrazidic acid (see P-65.2.1.4)
(not carbazic acid)



[benzo[1,2-*c*:3,4-*c*′]bis([1,2,5]oxadiazole)]-4-carboxylic acid (PIN)

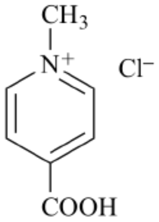


4,4′-methylenedi(cyclohexane-1-carboxylic acid) (PIN)

P-65.1.2.2.3 The prefixes ‘carboxy’ and ‘oxalo’

When another group is present that has priority for citation as suffix, for example, a free valence, or when all carboxylic acid groups cannot be described by a suffix, carboxylic acid groups, –COOH, are indicated by the preferred prefix ‘carboxy’ (also used in general nomenclature). The prefix ‘oxalo’ is recommended as the preferred prefix for –CO-CO-OH, but cannot be used to lengthen a carbon chain. In general nomenclature, the compound prefix ‘carboxycarbonyl’ may be used, but the compound prefix ‘carboxyformyl’ is not recommended.

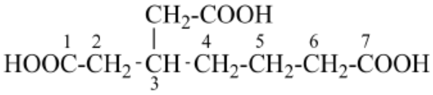
Examples:



4-carboxy-1-methylpyridin-1-ium chloride (PIN)

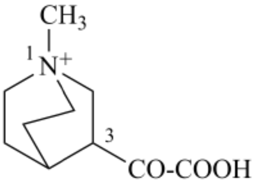
$\mathrm{–CH_2\text{-}CH_2\text{-}COOH}$

2-carboxyethyl (preferred prefix)



$$\mathrm{HOO\overset{1}{C}\text{-}\overset{2}{C}H_2\text{-}\underset{3}{\overset{\overset{CH_2\text{-}COOH}{|}}{C}}H\text{-}\overset{4}{C}H_2\text{-}\overset{5}{C}H_2\text{-}\overset{6}{C}H_2\text{-}\overset{7}{C}OOH}$$

3-(carboxymethyl)heptanedioic acid (PIN)



1-methyl-3-oxalo-1-azabicyclo[2.2.2]octan-1-ium (PIN)

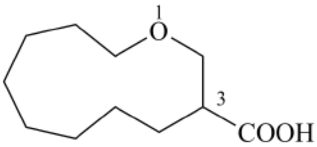
$$\mathrm{—\overset{1}{C}H_2\text{-}\overset{2}{C}H_2\text{-}\overset{3}{C}O\text{-}COOH}$$

3-carboxy-3-oxopropyl (preferred prefix)
(not 2-oxaloethyl)

P-65.1.2.3 Seniority order for numbering

When required, numbering is based on the seniority order given in P-14.4.

Examples:

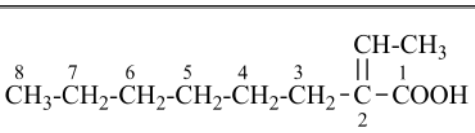


1-oxacycloundecane-3-carboxylic acid (PIN)

$$\mathrm{\overset{1}{C}H_3\text{-}\overset{2}{O}\text{-}CH_2\text{-}CH_2\text{-}\overset{5}{O}\text{-}CH_2\text{-}CH_2\text{-}\overset{8}{O}\text{-}CH_2\text{-}CH_2\text{-}\overset{11}{S}\text{-}CH_2\text{-}CH_2\text{-}\overset{14}{C}OOH}$$

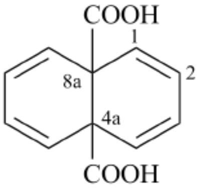
2,5,8-trioxa-11-thiatetradecan-14-oic acid (PIN)

Heteroatoms in chains are now considered to be an integral part of the parent hydride and as such they have seniority over suffixes for numbering (see P-14.4; see also P-15.4).

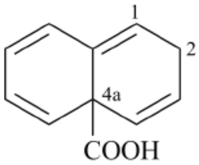


$$\mathrm{\overset{8}{C}H_3\text{-}\overset{7}{C}H_2\text{-}\overset{6}{C}H_2\text{-}\overset{5}{C}H_2\text{-}\overset{4}{C}H_2\text{-}\overset{3}{C}H_2\text{-}\underset{2}{\overset{\overset{CH\text{-}CH_3}{||}}{C}}\text{-}\overset{1}{C}OOH}$$

2-ethylideneoctanoic acid (PIN)
[not 2-hexylbut-2-enoic acid; see P-44.3, criterion (b)]



naphthalene-4a,8a-dicarboxylic acid (PIN; see P-58.2)
4a,8a-dihydronaphthalene-4a,8a-dicarboxylic acid



naphthalene-4a(2*H*)-carboxylic acid (PIN; see P-58.2)
2,4a-dihydronaphthalene-4a-carboxylic acid

P-65.1.2.4 Polyfunctional carboxylic acids

Systematic names of substituted carboxylic acids are formed by adding appropriate prefixes, such as ‘oxo’, ‘hydroxy’, ‘amino’, ‘imino’, ‘halo’, ‘nitro’, etc., to the name of the acid. Prefixes are not ranked as functional entities; they are cited in a name in alphabetical order (except for hydro/dehydro) which is also used to assign lowest locants when required.

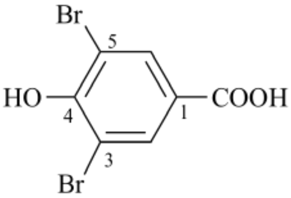
Examples:

$$\overset{6}{C}H_3\text{-}\overset{5}{C}O\text{-}\overset{4}{C}H_2\text{-}\overset{3}{C}H_2\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}OOH$$

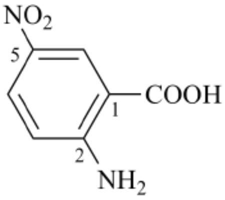
5-oxohexanoic acid (PIN)

$$H_2\overset{5}{N}\text{-}\overset{4}{C}H_2\text{-}\overset{3}{C}H_2\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}H_2\text{-}COOH$$

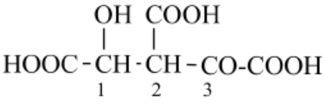
5-aminopentanoic acid (PIN)



3,5-dibromo-4-hydroxybenzoic acid (PIN)



2-amino-5-nitrobenzoic acid (PIN)
(not 5-nitroanthranilic acid;
anthranilic acid is not a retained name)



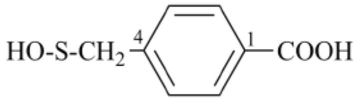
$$HOOC\text{-}\underset{1}{\overset{\overset{\displaystyle OH}{|}}{C}H}\text{-}\underset{2}{\overset{\overset{\displaystyle COOH}{|}}{C}H}\text{-}\underset{3}{C}O\text{-}COOH$$

1-hydroxy-3-oxopropane-1,2,3-tricarboxylic acid (PIN)
[not 3-hydroxy-1-oxopropane-1,2,3-tricarboxylic acid;
lowest locants are attributed to prefixes that are cited first, see P-14.4 (g)]

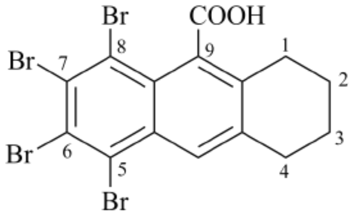
$(HO\text{-}CH_2\text{-}CH_2\text{-}O)_2CH\text{-}COOH$
bis(2-hydroxyethoxy)acetic acid (PIN)

$$CH_3\text{-}S\text{-}\overset{4}{C}H_2\text{-}\overset{3}{C}H_2\text{-}\overset{2}{C}O\text{-}\overset{1}{C}OOH$$

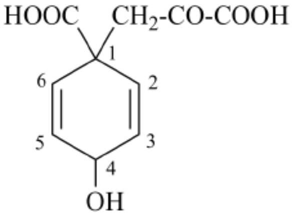
4-(methylsulfanyl)-2-oxobutanoic acid (PIN)
[not 4-(methylthio)-2-oxobutyric acid]



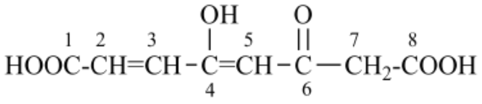
4-[(hydroxysulfanyl)methyl]benzoic acid (PIN)
[not 4-(sulfenomethyl)benzoic acid]



5,6,7,8-tetrabromo-1,2,3,4-tetrahydroanthracene-9-carboxylic acid (PIN)
(not 1,2,3,4-tetrabromo-5,6,7,8-tetrahydroanthracene-9-carboxylic acid
hydro/dehydro prefixes are given lowest possible locants before other detachable prefixes; see P-14.4)

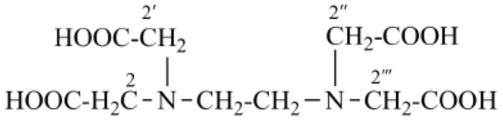


1-(2-carboxy-2-oxoethyl)-4-hydroxycyclohexa-2,5-diene-1-carboxylic acid (PIN)
1-carboxy-4-hydroxy-α-oxocyclohexa-2,5-dienepropanoic acid
(a conjunctive name, see P-15.6)



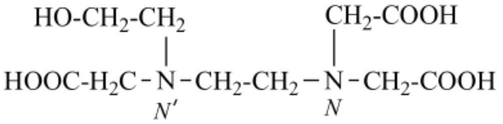
$$\text{HOOC-CH=CH-}\overset{\text{OH}}{\underset{4}{\text{C}}}\text{=CH-}\overset{\text{O}}{\underset{6}{\text{C}}}\text{-CH}_2\text{-COOH}$$

4-hydroxy-6-oxoocta-2,4-dienedioic acid (PIN)
(not 5-hydroxy-3-oxoocta-4,6-dienedioic acid;
unsaturation is senior to detachable prefixes for numbering)



$$(\text{HOOC-CH}_2)_2\text{N-CH}_2\text{-CH}_2\text{-N}(\text{CH}_2\text{-COOH})_2$$

2,2′,2″,2‴-(ethane-1,2-diyldinitrilo)tetraacetic acid (see P-15.3.2.1)
N,*N*′-(ethane-1,2-diyl)bis[*N*-(carboxymethyl)glycine]



$$(\text{HO-CH}_2\text{-CH}_2)(\text{HOOC-H}_2\text{C})\underset{N'}{\text{N}}\text{-CH}_2\text{-CH}_2\text{-}\underset{N}{\text{N}}(\text{CH}_2\text{-COOH})_2$$

N-(carboxymethyl)-*N*′-(2-hydroxyethyl)-*N*,*N*′-(ethane-1,2-diyl)diglycine
2,2′-({2-[(carboxymethyl)(2-hydroxyethyl)amino]ethyl}azanediyl)diacetic acid

P-65.1.3 Carboximidic, carbohydrazonic, carbohydroximic, and carbohydroxamic acids

P-65.1.3.1 Carboximidic acids

P-65.1.3.1.1 Substitutive nomenclature, suffix mode

The name of an acid in which the carbonyl oxygen atom of a carboxylic acid group has been replaced by =NH is formed by functional replacement nomenclature and the infix ‘imid(o)’ to modify the ‘ic acid’ or ‘oic acid’ ending of the retained name of an acid; or the ‘oic acid’ or ‘carboxylic acid’ suffix of a systematic name of an acid, to ‘imidic acid’ or ‘carboximidic acid’.

Preferred names of imidic acids are those derived from systematic substitutive preferred IUPAC names of carboxylic acids.

> The use of systematic substitutive names for imidic acids is a change for formic acid, acetic acid, benzoic acid, and oxalic acid.

Examples:

HC(=NH)-OH
methanimidic acid (PIN)
formimidic acid

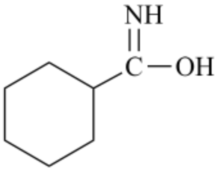
CH_3-C(=NH)-OH
ethanimidic acid (PIN)
acetimidic acid

C_6H_5-C(=NH)-OH
benzenecarboximidic acid (PIN)
benzimidic acid

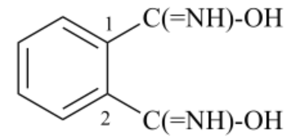
$\overset{4}{C}H_3\text{-}\overset{3}{C}H_2\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}(=NH)\text{-}OH$
butanimidic acid (PIN)
butyrimidic acid

$HO\text{-}\overset{4}{C}(=NH)\text{-}\overset{3}{C}H_2\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}(=NH)\text{-}OH$
butanediimidic acid (PIN)
succinimidic acid

HO-C(=NH)-C(=NH)-OH
ethanediimidic acid (PIN)
oxalimidic acid



cyclohexanecarboximidic acid (PIN)



benzene-1,2-dicarboximidic acid (PIN)
phthalimidic acid

P-65.1.3.1.2 Substitutive nomenclature, prefix mode

When another group is present that has seniority for citation as principal group, the following prefixes are used:

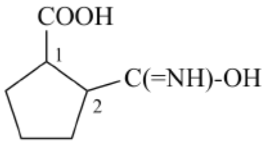
(1) the compound prefix '*C*-hydroxycarbonimidoyl' used to denote the acyl group –C(=NH)-OH is formed by concatenation based on the simple prefix carbonimidoyl, –C(=NH)–, derived from carbonimidic acid (see P-65.2.1.5);

(2) a combination of the simple prefixes 'hydroxy' and 'imino' at the end of a carbon chain is used in preferred IUPAC names rather than the compound prefix '*C*-hydroxycarbonimidoyl'.

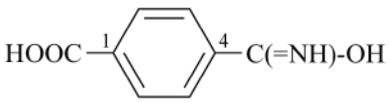
Note 1: The italicized letter '*C*' is used to avoid potential confusion with *N*-hydroxy substitution.

Note 2: The name carbonohydroximoyl, for –C(=NH)-OH, is not used to generate preferred IUPAC names.

Examples:

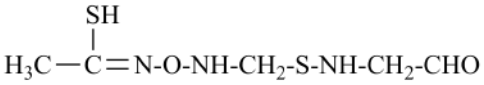


(1) 2-(*C*-hydroxycarbonimidoyl)cyclopentane-1-carboxylic acid (PIN)



(1) 4-(C-hydroxycarbonimidoyl)benzoic acid (PIN)

$HO\text{-}\overset{4}{C}(=NH)\text{-}\overset{3}{C}H_2\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}OOH$
(2) 4-hydroxy-4-iminobutanoic acid (PIN)
(1) 3-(*C*-hydroxycarbonimidoyl)propanoic acid



$$H_3C-\overset{\displaystyle SH}{\overset{|}{C}}=N\text{-}O\text{-}NH\text{-}CH_2\text{-}S\text{-}NH\text{-}CH_2\text{-}CHO$$

N-{[({[(2-oxoethyl)amino]sulfanyl}methyl)amino]oxy}ethanimidothioic acid (PIN)
(see P-65.1.5.2)

P-65.1.3.2 Carbohydrazonic acids

P-65.1.3.2.1 Substitutive nomenclature, suffix mode

The name of an acid in which the carbonyl oxygen atom of a carboxylic acid group has been replaced by $=NNH_2$ is formed by functional replacement nomenclature. The infix ‘hydrazon(o)’ is used to modify the ‘ic acid’ or ‘oic acid’ ending of the retained name of an acid; or the ‘oic acid’ or ‘carboxylic acid’ suffix of a systematic name of an acid is changed to ‘hydrazonic acid’ or ‘carbohydrazonic acid’.

Preferred IUPAC names for hydrazonic acids are those derived from systematic preferred IUPAC names of carboxylic acids.

> The use of systematic substitutive names for hydrazonic acids is a change for formic acid, acetic acid, benzoic acid, and oxalic acid.

Examples:

$H\text{-}C(=N\text{-}NH_2)\text{-}OH$
methanehydrazonic acid (PIN)
formohydrazonic acid

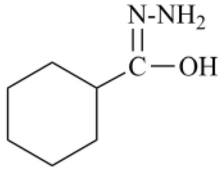
$CH_3\text{-}C(=N\text{-}NH_2)\text{-}OH$
ethanehydrazonic acid (PIN)
acetohydrazonic acid

$C_6H_5\text{-}C(=N\text{-}NH_2)\text{-}OH$
benzenecarbohydrazonic acid (PIN)
benzohydrazonic acid

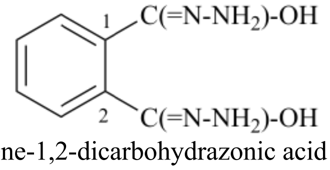
$\overset{4}{C}H_3\text{-}\overset{3}{C}H_2\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}(=N\text{-}NH_2)\text{-}OH$
butanehydrazonic acid (PIN)
butyrohydrazonic acid

$HO\text{-}\overset{4}{C}(=N\text{-}NH_2)\text{-}\overset{3}{C}H_2\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}(=N\text{-}NH_2)\text{-}OH$
butanedihydrazonic acid (PIN)
succinohydrazonic acid

$HO\text{-}C(=N\text{-}NH_2)\text{-}C(=N\text{-}NH_2)\text{-}OH$
ethanedihydrazonic acid (PIN)
oxalohydrazonic acid



cyclohexanecarbohydrazonic acid (PIN)



benzene-1,2-dicarbohydrazonic acid (PIN)
phthalohydrazonic acid

P-65.1.3.2.2 Substitutive nomenclature, prefix mode

When another group is present that has seniority for citation as principal group, the following prefixes are used:

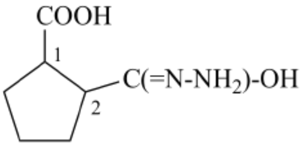
(1) the compound prefix ‘*C*-hydroxycarbonohydrazonoyl’ used to denote the acyl group $–C(=N\text{-}NH_2)\text{-}OH$ is formed by concatenation based on the simple prefix name carbonohydrazonoyl, $–C(=NNH_2)–$, derived from

carbonohydrazonic acid (see P-65.2.1.5)]. The substitutive name hydrazinylidene(hydroxy)methyl may be used in general nomenclature;

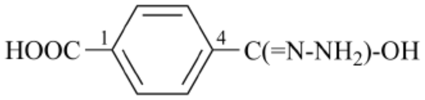
(2) the combination of the simple prefixes 'hydroxy' and 'hydrazinylidene' at the end of a carbon chain is used in preferred IUPAC names rather than the compound prefixes '*C*-hydroxycarbonohydrazonoyl' or 'hydrazinylidene(hydroxy)methyl'.

Note: The italicized letter '*C*' is used to avoid potential confusion with *N*-hydroxy substitution.

Examples:



(1) 2-(*C*-hydroxycarbonohydrazonoyl)cyclopentane-1-carboxylic acid (PIN)



(1) 4-(*C*-hydroxycarbonohydrazonoyl)benzoic acid (PIN)

$$\text{HO-}\overset{5}{\text{C}}\text{(=N-NH}_2\text{)-}\overset{4}{\text{C}}\text{H}_2\text{-}\overset{3}{\text{C}}\text{H}_2\text{-}\overset{2}{\text{C}}\text{H}_2\text{-}\overset{1}{\text{C}}\text{OOH}$$

(2) 5-hydrazinylidene-5-hydroxypentanoic acid (PIN)
(1) 4-(*C*-hydroxycarbonohydrazonoyl)butanoic acid

P-65.1.3.3 Carbohydroximic acids

P-65.1.3.3.1 Substitutive nomenclature, suffix mode

Acids in which the carbonyl oxygen atom of a carboxylic acid group has been replaced by =N-OH are named as *N*-hydroxy derivatives of imidic acids named as described in P-65.1.3.1. This method is used to generate preferred IUPAC names.

Note: The following former methodology is no longer used for preferred IUPAC names:

The name formed by modifying the '-oic acid' or '-carboxylic acid' suffix of a systematically named acid, or the '-ic acid' ending of the retained name of an acid to '-hydroximic acid' or '-carbohydroximic acid'. The letter 'o' is added for euphony between 'h' and a preceding consonant.

This former method may be still used in general nomenclature.

Examples:

$\text{CH}_3\text{-C(=N-OH)-OH}$
N-hydroxyethanimidic acid (PIN)
acetohydroximic acid

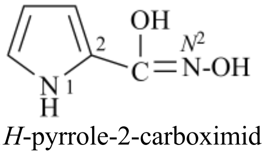
$\text{C}_6\text{H}_5\text{-C(=N-OH)-OH}$
N-hydroxybenzenecarboximidic acid (PIN)
benzohydroximic acid

$$\overset{4}{\text{C}}\text{H}_3\text{-}\overset{3}{\text{C}}\text{H}_2\text{-}\overset{2}{\text{C}}\text{H}_2\text{-}\overset{1}{\text{C}}\text{(=N-OH)-OH}$$

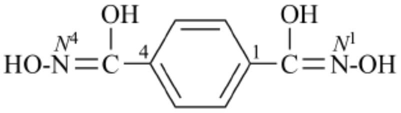
N-hydroxybutanimidic acid (PIN)
butyrohydroximic acid
butanohydroximic acid

$$\text{HO-}\overset{4}{\text{C}}\text{(=}\overset{N^4}{\text{N}}\text{-OH)-}\overset{3}{\text{C}}\text{H}_2\text{-}\overset{2}{\text{C}}\text{H}_2\text{-}\overset{1}{\text{C}}\text{(=}\overset{N^1}{\text{N}}\text{-OH)-OH}$$

N^1,N^4-dihydroxybutanediimidic acid
succinohydroximic acid
butanedihydroximic acid



N^2-hydroxy-1*H*-pyrrole-2-carboximidic acid (PIN)
pyrrole-2-carbohydroximic acid



N^1,N'^4-dihydroxybenzene-1,4-dicarboximidic acid (PIN)
terephthalohydroximic acid

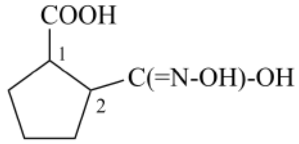
P-65.1.3.3.2 Substitutive nomenclature, prefix mode

When another group is present that has seniority for citation as principal group, the following prefixes are used:

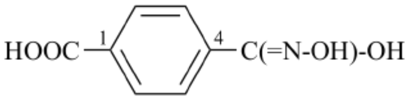
(1) '*C*,*N*-dihydroxycarbonimidoyl' to denote the group –C(=N-OH)-OH;

(2) the combination of the prefixes 'hydroxy' and 'hydroxyimino' at the end of a carbon chain is used in preferred IUPAC names rather than the prefix 'dihydroxycarbonimidoyl'.

Examples:



(1) 2-(*C*,*N*-dihydroxycarbonimidoyl)cyclopentane-1-carboxylic acid (PIN)



(1) 4-(*C*,*N*-dihydroxycarbonimidoyl)benzoic acid (PIN)

$$\mathrm{HO\text{-}\overset{5}{C}(=N\text{-}OH)\text{-}\overset{4}{C}H_2\text{-}\overset{3}{C}H_2\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}OOH}$$

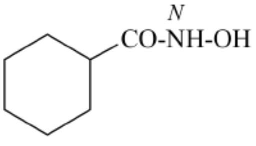
(2) 5-hydroxy-5-(hydroxyimino)pentanoic acid (PIN)
(1) 4-(*C*,*N*-dihydroxycarbonimidoyl)butanoic acid

P-65.1.3.4 Hydroxamic acids have the generic structure R-CO-NH-OH and are named as *N*-hydroxy amides (see P-66.1.1.3.2). The suffixes 'hydroxamic acid' and 'carbohydroxamic acid' are no longer recommended for preferred IUPAC names but may be used in general nomenclature.

Examples:

$$\mathrm{CH_3\text{-}CO\text{-}\overset{\mathit{N}}{N}H\text{-}OH}$$

N-hydroxyacetamide (PIN)
acetohydroxamic acid



N-hydroxycyclohexanecarboxamide (PIN)
cyclohexanecarbohydroxamic acid

P-65.1.4 Peroxycarboxylic acids

The general methodology for modifying acids expressed by suffixes by functional replacement nomenclature is to use modified suffixes in the same way as for unmodified acids. A major change and simplification is recommended, i.e., suffixes are always modified by infixes.

P-65.1.4.1 Peroxycarboxylic acids are named systematically using the following suffixes:

–(C)O-OOH peroxoic acid

–CO-OOH carboperoxoic acid

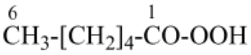
Retained names of carboxylic acids are modified by the prefix ‘peroxy’. Preferred IUPAC names are formed by functional replacement of systematic carboxylic acid names.

> The use of systematic substitutive names for peroxycarboxylic acids is a change for formic acid, acetic acid, benzoic acid, oxalic acid, and oxamic acid.

Examples:

HCO-OOH
methaneperoxoic acid (PIN)
peroxyformic acid
performic acid

CH_3-CO-OOH
ethaneperoxoic acid (PIN)
peroxyacetic acid
peracetic acid

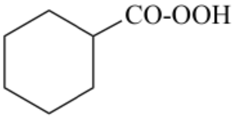


$\overset{6}{C}H_3\text{-}[CH_2]_4\text{-}\overset{1}{C}O\text{-}OOH$

hexaneperoxoic acid (PIN)

C_6H_5-CO-OOH
benzenecarboperoxoic acid (PIN)
peroxybenzoic acid
perbenzoic acid

H_2N-CO-CO-OOH
amino(oxo)ethaneperoxoic acid (PIN)
peroxyoxamic acid



cyclohexanecarboperoxoic acid (PIN)

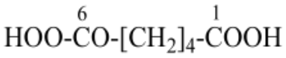
HOO-CO-CO-OOH
ethanediperoxoic acid (PIN)
diperoxyoxalic acid

P-65.1.4.2 When another group is present that has priority for citation as a suffix (see seniority of classes, P-41), the following prefixes are used:

(1) the simple functional replacement prefix ‘carbonoperoxoyl-’ or the compound prefix ‘hydroperoxycarbonyl-’, formed by concatenation based on the simple acyl group ‘carbonyl’, for >C=O (see P-65.2.1.5) is used to denote the acyl group –C(O)-OOH as a substituent; the prefix ‘carbonoperoxoyl’ is used in preferred IUPAC names, except as noted below in (2);

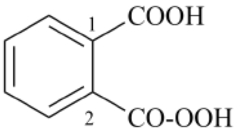
(2) the combination of the simple prefixes ‘hydroperoxy and oxo’ at the end of a carbon chain is used in preferred IUPAC names rather than the prefix ‘hydroperoxycarbonyl-’ or the prefix ‘carbonoperoxoyl-’.

Examples:

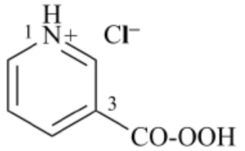


$HOO\text{-}\overset{6}{C}O\text{-}[CH_2]_4\text{-}\overset{1}{C}OOH$

(2) 6-hydroperoxy-6-oxohexanoic acid (PIN)
(1) 5-carbonoperoxoylpentanoic acid
5-(hydroperoxycarbonyl)pentanoic acid



(1) 2-carbonoperoxoylbenzoic acid (PIN)
(2) 2-(hydroperoxycarbonyl)benzoic acid
monoperoxyphthalic acid (see P-65.1.4.1)

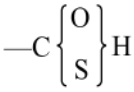


(1) 3-carbonoperoxoylpyridin-1-ium chloride (PIN)
3-(hydroperoxycarbonyl)pyridin-1-ium chloride

P-65.1.5 Chalcogen analogues of carboxylic acids

P-65.1.5.1 Functional replacement in systematic names of carboxylic acids

Replacement of oxygen atom(s) of a carboxylic acid group by another chalcogen is indicated by the affixes ‘thio’, ‘seleno’, and ‘telluro’. These names do not differentiate between tautomeric forms of mixed chalcogen acids; such nonspecificity may be shown in a structure such as:



$$—C\begin{Bmatrix}O\\S\end{Bmatrix}H \quad \text{or} \quad –C\{O/S\}H$$

In names, tautomeric groups in mixed chalcocarboxylic acids, such as –CO-SH or –CS-OH, –S(O)-SH or –S(S)-OH, are distinguished by prefixing italic element symbols, such as *O* or *S*, respectively, to the term ‘acid’, for example, thioic *S*-acid for –(C)O-SH and carbothioic *O*-acid for –CS-OH. Normally, these locants are omitted, because the exact position of chalcogen atoms is not known or important in acids; such letter locants are used mainly in naming esters.

When the position of chalcogen atoms is undetermined, the prefix for the unmodified acid, i.e. ‘carboxy’ for –COOH, is used and modified by functional replacement using prefixes, as in ‘thiocarboxy’ for –C{O/S}H, and is enclosed in parentheses to avoid the possibility of ambiguity. The order of seniority of these suffixes is fully described in Section P-43.

When the position of chalcogen atoms is known, combinations of prefixes such as ‘hydroxy- and sulfanylidene-’ or ‘sulfanyl- and oxo-’ are used in acyclic compounds. Compound prefixes such as ‘(hydroxycarbonothioyl)-’ and ‘(sulfanylcarbonyl)-’ are used when required as a substituent (see P-65.2.1.6). The compound prefixes are formed by concatenation using simple acyl prefixes derived from carbonic acids (see P-65.2.1.5)

The seniority order between acids and acids modified by functional replacement is discussed in P-43 and expressed in Table 4.3. In presence of unmodified acids cited as suffix, modified acids are cited as prefixes.

Examples:

CH_3-CH_2-CH_2-CH_2-CH_2-CS-OH
hexanethioic *O*-acid (PIN)

CH_3-CH_2-CH_2-CH_2-CH_2-C{S/Se}H
hexaneselenothioic acid (PIN)

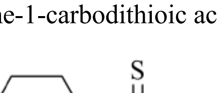
CH_3-CH_2-CH_2-CH_2-CH_2-CSe-SH
hexaneselenothioic *S*-acid (PIN)

H{S/O}C-CH_2-CH_2-CH_2-CH_2-C{O/S}H
hexanebis(thioic acid) (PIN)

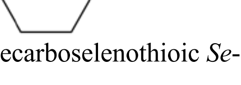
HS-SC-CH_2-CH_2-CH_2-CH_2-CS-SH
hexanebis(dithioic acid) (PIN)

CH_3-CH_2-CH_2-CH_2-CH_2-C{O/Se}H
hexaneselenoic acid (PIN)

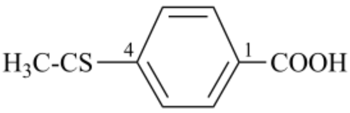
H{S/O}C-CH_2-CH_2-C{O/S}H
butanebis(thioic acid) (PIN)



piperidine-1-carbodithioic acid (PIN)



cyclohexanecarboselenothioic *Se*-acid (PIN)



4-(ethanethioyl)benzoic acid (PIN)
4-(thioacetyl)benzoic acid

$\overset{5}{\mathrm{H\{S/O\}C}}\text{-}\overset{4}{\mathrm{CH_2}}\text{-}\overset{3}{\mathrm{CH_2}}\text{-}\overset{2}{\mathrm{CH_2}}\text{-}\overset{1}{\mathrm{CH_2}}\text{-COOH}$

5-(thiocarboxy)pentanoic acid (PIN)

$\text{HS-}\overset{4}{\mathrm{CO}}\text{-}\overset{3}{\mathrm{CH_2}}\text{-}\overset{2}{\mathrm{CH_2}}\text{-}\overset{1}{\mathrm{COOH}}$

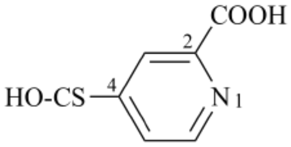
4-oxo-4-sulfanylbutanoic acid (PIN)
3-(sulfanylcarbonyl)propanoic acid

$\mathrm{HO\text{-}CS\text{-}CH_2\text{-}CH_2\text{-}COOH}$

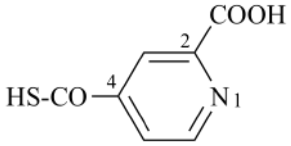
4-hydroxy-4-sulfanylidenebutanoic acid (PIN)

HS-CO-COOH

oxo(sulfanyl)acetic acid (PIN)



4-(hydroxycarbonothioyl)pyridine-2-carboxylic acid (PIN)



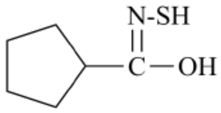
4-(sulfanylcarbonyl)pyridine-2-carboxylic acid (PIN)

$\mathrm{CH_3\text{-}CH_2\text{-}C(=NH)\text{-}SH}$

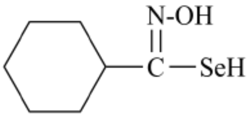
propanimidothioic acid (PIN)

$\mathrm{CH_3\text{-}CH_2\text{-}CH_2\text{-}C(=NNH_2)\text{-}SeH}$

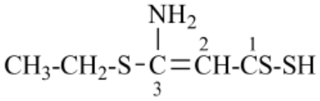
butanehydrazonoselenoic acid (PIN)



N-sulfanylcyclopentanecarboximidic acid (PIN)



N-hydroxycyclohexanecarboximidoselenoic acid (PIN)



$\mathrm{CH_3\text{-}CH_2\text{-}S\text{-}\overset{NH_2}{\underset{3}{C}}{=}\overset{2}{C}H\text{-}\overset{1}{C}S\text{-}SH}$

3-amino-3-(ethylsulfanyl)prop-2-ene(dithioic acid) (PIN)

P-65.1.5.2 Functional replacement in retained names of carboxylic acids

Preferred names of chalcogen analogues of monocarboxylic acids are formed using the suffixes ‘thioic acid’, ‘selenoic acid’, ‘telluroic acid’ or ‘carbothioic acid’, ‘carboselenoic acid’, ‘carbotelluroic acid’ and names of appropriate parent hydrides, even in the case of formic acid, acetic acid, and benzoic acid.

The use of systematic substitutive names for chalcogen analogues of monocarboxylic acids is a change for formic acid, acetic acid, benzoic acid, oxalic acid, and oxamic acid.

Chalcogen analogues of monocarboxylic acids with retained names may also be named by placing the prefix ‘thio’, ‘seleno’, or ‘telluro’ in front of the name of the acid.

Chalcogen analogues of dicarboxylic acids are named systematically; retained names are not used for naming chalcogen analogues of dicarboxylic acids.

The symbols *O*, *S*, *Se*, and *Te* are used to specify the structure of the acid, as indicated in P-65.1.5.1.

Examples:

$\mathrm{CH_3\text{-}CS\text{-}OH}$
ethanethioic *O*-acid (PIN)
thioacetic *O*-acid

$\mathrm{C_6H_5\text{-}C\{O/Se\}H}$
benzenecarboselenoic acid (PIN)
selenobenzoic acid

$\mathrm{HCO\text{-}SH}$
methanethioic *S*-acid (PIN)
thioformic *S*-acid

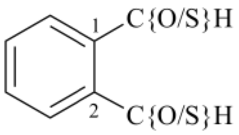
$\mathrm{H_2N\text{-}CO\text{-}CO\text{-}C\{O/S\}H}$
3-amino-2,3-dioxopropanethioic acid (PIN)

$\mathrm{H\{S/O\}\overset{4}{C}\text{-}\overset{3}{C}H_2\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}H_2\text{-}COOH}$
4-(thiocarboxy)butanoic acid (PIN)
(not thioglutaric acid)

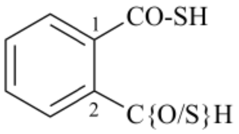
$\mathrm{HS\text{-}\overset{4}{C}O\text{-}\overset{3}{C}H_2\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}OOH}$
4-oxo-4-sulfanylbutanoic acid (PIN)
(not thiosuccinic acid)

$\mathrm{H\{S/O\}C\text{-}COOH}$
(thiocarboxy)formic acid
(see P-65.1.8.2)

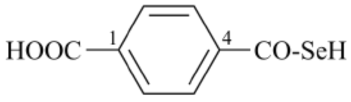
$\mathrm{HO\text{-}CS\text{-}COOH}$
hydroxy(sulfanylidene)acetic acid (PIN)



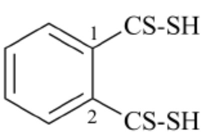
benzene-1,2-dicarbothioic acid (PIN)
(not 1,2-dithiophthalic acid)



2-(thiocarboxy)benzene-1-carbothioic *S*-acid (PIN)
(not 1,2-dithiophthalic *S*-acid)



4-(selanylcarbonyl)benzoic acid (PIN)
(not selenoterephthalic *Se*-acid)



benzene-1,2-dicarbodithioic acid (PIN)
(not tetrathiophthalic acid)

$\mathrm{HS\text{-}CS\text{-}CS\text{-}SH}$
ethanebis(dithioic acid) (PIN)
(not tetrathiooxalic acid)

P-65.1.5.3 Functional replacement in peroxycarboxylic acids

Peroxy acid suffixes can be modified by S, Se, and Te using functional replacement nomenclature. Italic prefixes in front of the term ‘acid’ are used for specificity, where necessary (see Table 4.3 for more suffixes modified by functional replacement and their seniority order). Preferred names are all formed by using appropriate suffixes and parent hydrides, even in the case of derivatives of formic acid, acetic acid, and benzoic acid.

> The use of systematic substitutive names for chalcogen analogues of peroxycarboxylic acids is a change for formic acid, acetic acid, benzoic acid, and oxalic acid.

Examples:

–(C)O-OSH (thioperoxoic) *OS*-acid (preferred suffix)

–(C)Se-SSH (dithioperoxo)selenoic acid (preferred suffix)

–CO-SOH carbo(thioperoxoic) *SO*-acid (preferred suffix)

–CS-OOH carboperoxothioic acid (preferred suffix)

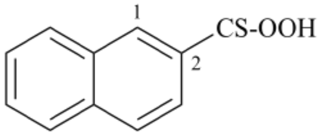
–COS_2H dithiocarboperoxoic acid (preferred suffix; location of sulfur atom unknown)

The recommended suffixes, and their seniority order, are fully discussed in Section P-43.

Examples:

CH_3-CO-OSH
ethane(thioperoxoic) *OS*-acid (PIN)
(not peroxythioacetic *OS*-acid)

C_6H_5-CO-SOH
benzenecarbo(thioperoxoic) *SO*-acid (PIN)
(not peroxothiobenzoic *SO*-acid)



naphthalene-2-carboperoxothioic acid (PIN)
(not peroxythio-2-naphthoic acid)

Compound prefixes, such as ‘sulfanyloxy’ and ‘oxo’ and ‘hydroxysulfanyl’ and ‘sulfanylidene’ at the end of acyclic chains are used to generate preferred IUPAC names. Appropriate prefixes constructed by concatenation based on simple acyl groups derived from carbonic and related acids (see P-65.2.1.5) are also used in preferred IUPAC names. Letter locants such as ‘*SO*’ and ‘*OS*’ are required to specify structures of thioperoxy groups (see also P-63.4.2.2).

Prefixes derived by functional replacement nomenclature have only limited use because there is no accepted method to unambiguously describe precise structures of thioperoxy groups.

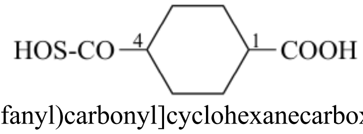
Examples:

$\text{HS-O-}\overset{4}{\text{C}}\text{S-}\overset{3}{\text{C}}\text{H}_2\text{-}\overset{2}{\text{C}}\text{H}_2\text{-}\overset{1}{\text{C}}\text{OOH}$
4-sulfanylidene-4-(sulfanyloxy)butanoic acid (PIN)
3-[(*SO*-thiohydroperoxy)carbonothioyl]propanoic acid (see P-63.4.2.2)
[not 3-carbono(thioperoxo)thioylpropanoic acid; ambiguous name]

$\text{HOS}_2\overset{4}{\text{C}}\text{-}\overset{3}{\text{C}}\text{H}_2\text{-}\overset{2}{\text{C}}\text{H}_2\text{-}\overset{1}{\text{C}}\text{OOH}$
3-(dithiocarbonoperoxoyl)propanoic acid (PIN)
(location of sulfur atoms unknown)

HOS_2C-COOH
(dithiocarbonoperoxoyl)formic acid (PIN)
(location of sulfur atoms unkown)

HOS-CO-COOH
(hydroxysulfanyl)oxoacetic acid (PIN)



4-[(hydroxysulfanyl)carbonyl]cyclohexanecarboxylic acid (PIN)
4-[(*OS*-thiohydroperoxy)carbonyl]cyclohexanecarboxylic acid

P-65.1.6 Amic, anilic, and aldehydic acids

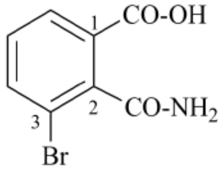
Amic acids are compounds containing both a carboxy, –COOH, and a carboxamide, $–CONH_2$, group; similarly, anilic and aldehydic acids include both a carboxy group and a carboxanilide, $–CO\text{-}NH\text{-}C_6H_5$, or formyl, –CHO, group, respectively. The endings ‘amic acid’, ‘anilic acid’, and ‘aldehydic acid’ can only be used in general nomenclature to name modified dicarboxylic acids having retained names. Preferred IUPAC names are all formed systematically using preferred names of acids and appropriate prefixes.

P-65.1.6.1 Amic acids

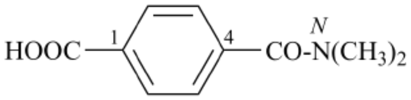
When a dicarboxylic acid has a retained name (see P-65.1.1) and when one of its carboxy groups is replaced by a carboxamide group, $–CO\text{-}NH_2$, the resulting structure is called an amic acid and, in general nomenclature may be named by replacing the ending ‘ic acid’ of the name of the dicarboxylic acid by the ending ‘amic acid’. The case of oxalic acid is special; substitution is not possible for the acid, but substitution is allowed for the derived amic acid, ‘oxamic acid’ but no ‘*N*’ locamnts are necessary. The name ‘oxamic acid’ (a contraction of ‘oxalamic acid’) is retained for $H_2N\text{-}CO\text{-}COOH$ and is the preferred IUPAC name.

The prefix ‘carbamoyl’ is preferred to ‘aminocarbonyl’ for naming amic acids systematically. The combination of the prefixes ‘amino’ and ‘oxo’ is used for describing the $–CO\text{-}NH_2$ at the end of an acyclic chain in preferred IUPAC names

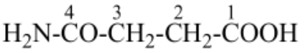
Examples:



3-bromo-2-carbamoylbenzoic acid (PIN)
2-(aminocarbonyl)-3-bromobenzoic acid



4-(dimethylcarbamoyl)benzoic acid (PIN)
4-[(dimethylamino)carbonyl]benzoic acid
N,*N*-dimethylterephthalamic acid


$H_2N\text{-}\overset{4}{C}O\text{-}\overset{3}{C}H_2\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}OOH$

4-amino-4-oxobutanoic acid (PIN)
3-carbamoylpropanoic acid
3-(aminocarbonyl)propanoic acid
succinamic acid

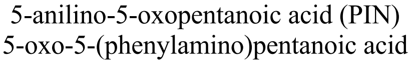
$H_2N\text{-}CO\text{-}COOH$
oxamic acid (PIN; a retained name)
(not oxalamic acid)

P-65.1.6.2 Anilic acids

N-Phenyl derivatives of amic acids are called ‘anilic acids’ and in general nomenclature are named by changing an ‘amic acid’ ending to ‘anilic acid’. Substitution on the nitrogen atom is indicated by the locant *N*, even if no substitution is allowed on the parent acid. Anilic acids may also be named as *N*-substituted amic acids. The locants for substituents on the *N*-phenyl ring are primed numbers.

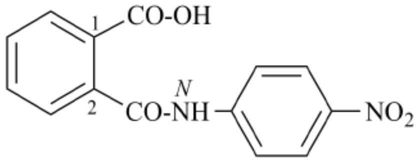
The combination of the prefixes ‘anilino’ and ‘oxo’ is used for describing $–CO\text{-}NH\text{-}C_6H_5$ at the end of an acyclic chain resulting in preferred IUPAC names

Examples:


$C_6H_5\text{-}NH\text{-}\overset{5}{C}O\text{-}\overset{4}{C}H_2\text{-}\overset{3}{C}H_2\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}OOH$

5-anilino-5-oxopentanoic acid (PIN)
5-oxo-5-(phenylamino)pentanoic acid
4-(phenylcarbamoyl)butanoic acid
N-phenylglutaramic acid
glutaranilic acid

C_6H_5-NH-CO-COOH
anilino(oxo)acetic acid (PIN)
oxalanilic acid

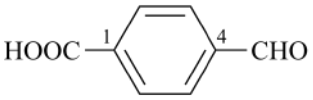


2-[(4-nitrophenyl)carbamoyl]benzoic acid (PIN)
N-(4-nitrophenyl)phthalamic acid
4′-nitrophthalanilic acid

P-65.1.6.3 Aldehydic acids

When a dicarboxylic acid has a retained name (see P-65.1.1) and when one of its carboxy groups is replaced by a formyl group, –CHO (see P-65.1.7.2.1), the resulting structure is called an aldehydic acid and, in general nomenclature may be named by replacing the ending ‘ic acid’ of the name of the dicarboxylic acid by the ending ‘aldehydic acid’. Preferred IUPAC names for aldehydic acids derived from all dicarboxylic acids are constructed systematically. The prefix ‘formyl’ is used in preferred IUPAC names, except for a –CHO group at the end of an acyclic chain, which is designated by the prefix ‘oxo’.

Examples:



4-formylbenzoic acid (PIN)
terephthalaldehydic acid

$\mathrm{OH}\overset{4}{\mathrm{C}}\text{-}\overset{3}{\mathrm{C}}\mathrm{H_2}\text{-}\overset{2}{\mathrm{C}}\mathrm{H_2}\text{-}\overset{1}{\mathrm{C}}\mathrm{OOH}$
4-oxobutanoic acid (PIN)
3-formylpropanoic acid
succinaldehydic acid

OCH-CO-OH
oxoacetic acid (PIN)
(not glyoxylic acid)

P-65.1.7 Acyl groups derived from carboxylic and related acids

P-65.1.7.1 Definitions and name formation
P-65.1.7.2 Acyl groups derived from carboxylic acids having retained names that are preferred IUPAC names (see P-65.1.1.1), i.e., carboacyl groups
P-65.1.7.3 Acyl groups derived from carboxylic acids with names retained only for general nomenclature (see P-65.1.1.2)
P-65.1.7.4 Acyl groups derived from systematically named carboxylic acids
P-65.1.7.5 Mixed acyl groups

P-65.1.7.1 Definitions and name formation

Carboacyl groups are R-CO–, –OC-R-CO–, or –OC-R-[R′-CO-]$_x$-R″-CO– groups and their functional replacement analogues, where R, R′, and R″ are chains, rings, or ring systems, derived from carboxylic acids by the removal of the hydroxy group from each carboxylic acid group that is expressed by the suffix, and x = 1, 2, 3, etc.

Systematic names for carboacyl groups and their functional replacement analogues are given in the following subsections. Compound substitutive names for acyclic acyl groups, such as ‘1-oxopropyl’ and ‘1-iminoethyl’ for CH_3-CH_2-CO– and CH_3-C(=NH)–, respectively, are included for use in general nomenclature.

P-65.1.7.2 Acyl groups derived from carboxylic acids having retained names that are preferred IUPAC names (see P-65.1.1.1), i.e., carboacyl groups.

The name of a monovalent or divalent carboacyl groups derived by removal of the –OH group from each carboxy group of a carboxylic acid or functional replacement analogue denoted by an ‘oic acid’ or ‘ic acid’ suffix or having a trivial name is derived from the name of the corresponding acid by changing the ‘oic acid’ or ‘ic acid’ ending to ‘oyl’ or ‘yl’. The general rule that the ending of all acyl group prefixes be ‘oyl’, proposed years ago, has not been regularly followed. This rule is fully implemented in these recommendations, but some traditional exceptions are maintained.

Carboacyl groups derived from acids named by means of the suffix ‘carboxylic acid’ are named by changing the suffix ‘carboxylic acid’ to ‘carbonyl’. Acyl groups derived from functional replacement analogues are named by changing the suffixes ‘carbothioic acid’ to ‘carbothioyl’ (and likewise for the selenium and tellurium analogues); ‘carboximidic acid’ to ‘carboximidoyl’; ‘carbohydrazonic acid’ to ‘carbohydrazonoyl’; and ‘carbohydroximic acid’ to ‘carbohydroximoyl’.

P-65.1.7.2.1 Acyl groups from the carboxylic acids that have retained names used as preferred IUPAC names (see P-65.1.1.1)

Examples:

CH_3-CO–
acetyl (preferred prefix)
ethanoyl
1-oxoethyl

HCO–
formyl (preferred prefix)
methanoyl
oxomethyl

C_6H_5-CO–
benzoyl (preferred prefix)
benzenecarbonyl
oxo(phenyl)methyl

–CO-CO–
oxalyl (preferred prefix)
ethanedioyl
dioxoethanediyl

HO-CO-CO–
oxalo (preferred prefix)
carboxycarbonyl
[not carboxyformyl;
not hydroxy(oxo)acetyl]

P-65.1.7.2.2 Acyl groups corresponding to the carboximidic, carbohydrazonic, carbohydroximic, and carbohydroxamic acids described in P-65.1.3.

The use of systematically derived acyl groups from imidic, hydrazonic, hydroximic, and hydroxamic acids is a changes for formic, acetic, benzoic, and oxalic acids.

Examples:

CH_3-C(=NH)–
ethanimidoyl (preferred prefix)
acetimidoyl
1-iminoethyl

HC(=NH)–
methanimidoyl (preferred prefix)
formimidoyl
iminomethyl

C_6H_5-C(=NH)–
benzenecarboximidoyl (preferred prefix)
benzimidoyl
imino(phenyl)methyl

–C(=NH)-C(=NH)–
ethanediimidoyl (preferred prefix)
oxalimidoyl
diiminoethanediyl

HC(=NNH_2)–
methanehydrazonoyl (preferred prefix)
formohydrazonoyl
hydrazinylidenemethyl

CH_3-C(=NNH_2)–
ethanehydrazonoyl (preferred prefix)
acetohydrazonoyl
1-hydrazinylideneethyl

C_6H_5-C(=N-OH)–
N-hydroxybenzenecarboximidoyl (preferred prefix)
N-hydroxybenzimidoyl
benzenecarbohydroximoyl

P-65.1.7.2.3 Chalcogen analogues of acyl groups corresponding to carboxylic acids having retained names that are preferred IUPAC names are named systematically using the infixes of functional replacement nomenclature; these names are preferred IUPAC names.

The use of systematically derived acyl groups from chalcogen analogues of carboxylic acids is a change for formic, acetic, benzoic, and oxalic acids.

Examples:

CH_3-CSe–
ethaneselenoyl (preferred prefix)
selenoacetyl
1-selanylideneethyl

HCS–
methanethioyl (preferred prefix)
thioformyl
sulfanylidenemethyl

C_6H_5-CS–
benzenecarbothioyl (preferred prefix)
thiobenzoyl

–CS-CS–
ethanebis(thioyl) (preferred prefix)
dithiooxalyl
bis(sulfanylidene)ethanediyl

P-65.1.7.2.4 Acyl groups and substituent groups derived from oxalic acid

Examples:

OCH-CO–
oxoacetyl (from oxoacetic acid, P-65.1.6.3)
(preferred prefix)

Cl-CO-CO–
chloro(oxo)acetyl (preferred prefix)
chlorooxalyl

HO-CO-CS–
carboxymethanethioyl (preferred prefix)

HO-CS-CO–
hydroxy(sulfanylidene)acetyl (preferred prefix)
(not 2-thiooxalo;
not 2-hydroxy-2-thiooxalyl)

HO-CS-CS–
hydroxy(sulfanylidene)ethanethioyl (preferred prefix)
hydroxybis(sulfanylidene)ethyl
(not 1,2-dithiooxalyl)

HS-CS-CS–
sulfanyl(sulfanylidene)ethanethioyl (preferred prefix)
trithiooxalo

HO-CO-CO-O–
oxalooxy (preferred prefix)
(carboxycarbonyl)oxy

HO-CO-CO-NH–
oxaloamino (preferred prefix)
(carboxycarbonyl)amino

HO-CO-CO-S–
oxalosulfanyl (preferred prefix)
(carboxycarbonyl)sulfanyl

HO-CO-CS-S–
(carboxymethanethioyl)sulfanyl (preferred prefix)

P-65.1.7.3 Acyl groups derived from carboxylic acids with names retained only for general nomenclature (see P-65.1.1.2)

P-65.1.7.3.1 Traditional names are maintained for acyl groups derived from acids having retained names for use only in general nomenclature (see P-65.1.1.2); substitution on acyl groups is identical to that of acids. The rule of having acyl groups ending in 'oyl' is applied, with certain exceptions that end in 'yl'. The following exceptions below are limiting. Preferred IUPAC names are systematic substitutive names.

Examples:

CH_3-CH_2-CH_2-CO–
butyryl
butanoyl (preferred prefix))
1-oxobutyl

CH_3-CH_2-CO–
propionyl
propanoyl (preferred prefix)
1-oxopropyl

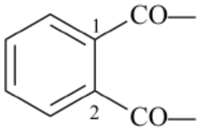
–OC-CH_2-CO–
malonyl
propanedioyl (preferred prefix)
1,3-dioxopropane-1,3-diyl

–CO-CH_2-CH_2-CO–
succinyl
butanedioyl (preferred prefix)
1,4-dioxobutane-1,4-diyl

–OC-[CH_2]$_3$-CO–
glutaryl
pentanedioyl (preferred prefix)
1,5-dioxopentane-1,5-diyl

CH_2=CH-CO–
acryloyl
prop-2-enoyl (preferred prefix)
1-oxoprop-2-en-1-yl

CH_2=C(CH_3)-CO–
methacryloyl
2-methylprop-2-enoyl (preferred prefix)
2-methyl-1-oxoprop-2-en-1-yl



phthaloyl
benzene-1,2-dicarbonyl (preferred prefix)
1,2-phenylenebis(oxomethylene)

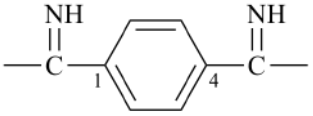
P-65.1.7.3.2 Acyl groups derived from imidic, hydrazonic, and hydroximic acids with retained names for use only in general nomenclature are named by changing the 'ic acid' ending of the names described in P-65.1.3 into 'oyl'.

Examples:

CH_3-CH_2-C(=NH)–
propionimidoyl
propanimidoyl (preferred prefix)
1-iminopropyl

CH_2=CH-C(=NNH_2)–
acrylohydrazonoyl
prop-2-enehydrazonoyl (preferred prefix)
1-hydrazinylideneprop-2-en-1-yl

–(HN=)C-CH_2-CH_2-C(=NH)–
succinimidoyl
butanediimidoyl (preferred prefix)
1,4-diiminobutane-1,4-diyl



terephthalimidoyl
benzene-1,4-dicarboximidoyl (preferred prefix)
1,4-phenylenebis(iminomethylene)

P-65.1.7.3.3 Chalcogen analogues of acyl groups derived from acids having retained names that are used only in general nomenclature are named using prefixes expressing functional replacement

Names of acyl groups derived from monocarboxylic acids are modified by prefixes expressing functional replacement by =S, =Se, and =Te. Acyl group prefixes corresponding to dicarboxylic acids are formed systematically, in accordance with Rule P- 65.1.7.4.

Examples:

CH_3-CH_2-CS–
thiopropionyl
propanethioyl (preferred prefix)
1-sulfanylidenepropyl

CH_2=CH-CSe–
selenoacryloyl
prop-2-eneselenoyl (preferred prefix)
1-selanylideneprop-2-en-1-yl

HS-CS-CS–
sulfanyl(sulfanylidene)ethanethioyl (preferred prefix)
2-sulfanyl-1,2-bis(sulfanylidene)ethyl
trithiooxalo

P-65.1.7.4 Acyl groups derived from systematically named carboxylic acids

P-65.1.7.4.1 The name of a monovalent or divalent acyl group formed by removal of the -OH group from each carboxy group of a carboxylic acid denoted by an ‘oic acid’ suffix is derived from the name of the corresponding acid by changing the ending ‘oic acid’ to ‘oyl’. Names of acyl groups derived from carboxylic acids modified by functional replacement are all denoted by the ending ‘oyl’.

Examples:

$\overset{3}{\mathrm{C}}\mathrm{H_3}\text{-}\overset{2}{\mathrm{C}}\mathrm{H_2}\text{-}\overset{1}{\mathrm{C}}\mathrm{O}—$
propanoyl (preferred prefix)
propionyl
1-oxopropyl

$—\mathrm{O}\overset{10}{\mathrm{C}}\text{-}[\mathrm{CH_2}]_8\text{-}\overset{1}{\mathrm{C}}\mathrm{O}—$
decanedioyl (preferred prefix)
1,10-dioxodecane-1,10-diyl

$\overset{4}{\mathrm{C}}\mathrm{H_3}\text{-}\overset{3}{\mathrm{C}}\mathrm{H_2}\text{-}\overset{2}{\mathrm{C}}\mathrm{H_2}\text{-}\overset{1}{\mathrm{C}}(\mathrm{=NH})—$
butanimidoyl (preferred prefix)
butyrimidoyl
1-iminobutyl

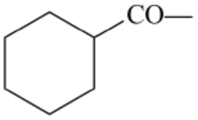
$—\overset{3}{\mathrm{C}}(\mathrm{=NH})\text{-}\overset{2}{\mathrm{C}}\mathrm{H_2}\text{-}\overset{1}{\mathrm{C}}(\mathrm{=NH})—$
propanediimidoyl (preferred prefix)
malonimidoyl
1,3-diiminopropane-1,3-diyl

CH_3-CH_2-CS–
propanethioyl (preferred prefix)
thiopropionyl
1-sulfanylidenepropyl
1-thioxpropyl

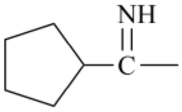
–CS-CH_2-CH_2-CS–
butanebis(thioyl) (preferred prefix)
1,4-bis(sulfanylidene)butane-1,4-diyl
1,4-dithioxobutane-1,4-diyl
(not dithiosuccinyl)

P-65.1.7.4.2 Acyl groups derived from an acid named by means of the suffix ‘carboxylic acid’ are named by changing the ‘carboxylic acid’ suffix to the suffix ‘carbonyl’. Similarly, the suffix ‘carbothioic acid’ is changed to ‘carbothioyl’; the suffix ‘carboselenoic acid’ is changed to ‘carboselenoyl’; the suffix ‘carbotelluroic acid’ is changed to ‘carbotelluroyl’; the suffix ‘carboximidic acid’ is changed to ‘carboximidoyl’; and the suffix ‘carbohydrazonic acid’ is changed to ‘carbohydrazonoyl’.

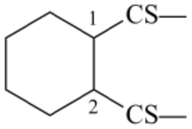
Examples:



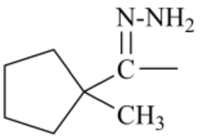
cyclohexanecarbonyl (preferred prefix)
cyclohexylcarbonyl
cyclohexyl(oxo)methyl



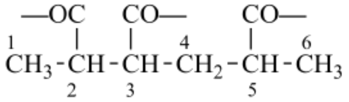
cyclopentanecarboximidoyl (preferred prefix)
cyclopentylcarbonimidoyl
cyclopentyl(imino)methyl



cyclohexane-1,2-dicarbothioyl (preferred prefix)

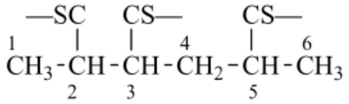


1-methylcyclopentane-1-carbohydrazonoyl (preferred prefix)
hydrazinylidene(1-methylcyclopentyl)methyl



$$\overset{1}{CH_3}\text{-}\underset{2}{\overset{\text{—OC}}{CH}}\text{-}\underset{3}{\overset{\text{CO—}}{CH}}\text{-}\overset{4}{CH_2}\text{-}\underset{5}{\overset{\text{CO—}}{CH}}\text{-}\overset{6}{CH_3}$$

hexane-2,3,5-tricarbonyl (preferred prefix)
hexane-2,3,5-triyltris(oxomethylene)
hexane-2,3,5-tris(carbonyl)



$$\overset{1}{CH_3}\text{-}\underset{2}{\overset{\text{—SC}}{CH}}\text{-}\underset{3}{\overset{\text{CS—}}{CH}}\text{-}\overset{4}{CH_2}\text{-}\underset{5}{\overset{\text{CS—}}{CH}}\text{-}\overset{6}{CH_3}$$

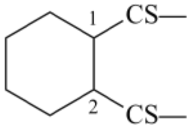
hexane-2,3,5-tricarbothioyl (preferred prefix)
hexane-2,3,5-triyltris(sulfanylidenemethylene)
hexane-2,3,5-triyltris(thioxomethylene)

P-65.1.7.4.3 Acyl groups derived from dicarboxylic acids with retained names modified by functional replacement by =S, =Se, and =Te are formed systematically, as described in P-65.1.7.4.2.

Examples:

$$\text{—}\overset{4}{CS}\text{-}\overset{3}{CH_2}\text{-}\overset{2}{CH_2}\text{-}\overset{1}{CS}\text{—}$$

butanebis(thioyl) (preferred prefix)
(not dithiosuccinyl)
1,4-bis(sulfanylidene)butane-1,4-diyl

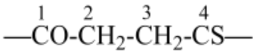


benzene-1,2-dicarbothioyl (preferred prefix)
(not dithiophthaloyl)
1,2-phenylenebis(sulfanylidenemethylene)
1,2-phenylenebis(thioxomethylene)

P-65.1.7.5 Mixed acyl groups

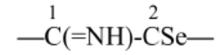
Mixed acyl groups of the type –(C=X)-$[CH_2]_x$-(C=Y)– are named by substitution of alkanediyl substituent groups.

Examples:



$$—\overset{1}{C}O\text{-}\overset{2}{C}H_2\text{-}\overset{3}{C}H_2\text{-}\overset{4}{C}S—$$

1-oxo-4-sulfanylidenebutane-1,4-diyl (preferred prefix)



$$—\overset{1}{C}(=NH)\text{-}\overset{2}{C}Se—$$

1-imino-2-selanylideneethane-1,2-diyl (preferred prefix)

P-65.1.8 Formic acid

For the purpose of organic nomenclature, formic acid is considered to be a monocarboxylic acid (see P-65.1). It is a retained name, treated like acetic acid, can be functionalized leading to salts, esters, and anhydrides, and forms an acyl group that is used as a substituent group. Functional replacement analogues are named systematically, for example, methanethioic acid and methanimidic acid. The hydrogen atom attached to carbon is substitutable under specific conditions that are described in P-65.1.8.1, P- 65.1.8.2, and P-65.1.8.3.

P-65.1.8.1 Substitution of the hydrogen atom of formic acid by the following atoms or groups is not recommended:

–OOH, –SH, –SeH, –TeH, –F, –Cl, –Br, –I, $–N_3$, –NC, –CN, –NCO, –NCS, –NCSe, –NCTe, $–NH_2$, $–NH\text{-}NH_2$

Names for such structures are derived from carbonic acid by functional replacement nomenclature (see P-65.2.1.4) and are preferred IUPAC names and used in general nomenclature:

Note: Substitution of the hydrogen atom of formic acid by $–NH\text{-}NH_2$ leads to a structure named by the suffix carboxylic acid attached to the parent hydride hydrazine (see P-68.3.1.2). A carboxylic acid named by means of a suffix is senior to a derivative of carbonic acid formed by functional replacement (see P-41).

Examples:

$H_2N\text{-}NH\text{-}COOH$
hydrazinecarboxylic acid (PIN)
carbonohydrazidic acid (see P-65.2.1.4)
(not carbazic acid)

Cl-COOH
carbonochloridic acid (PIN)
(not chloroformic acid)

HS-COOH
carbonothioic *S*-acid (PIN)
(not sulfanylformic acid)

P-65.1.8.2 Substitution of the hydrogen atom of formic acid is permitted when substituent groups are other than those cited in P-65.1.8.1.

Examples:

$O_2N\text{-}COOH$
nitroformic acid (PIN)

H{S/O}C-COOH
(thiocarboxy)formic acid (PIN, see P-65.1.5.2)

P-65.1.8.3 Acyl groups derived from formic acid are formed as described in P-65.1.7.2 and compound prefixes are formed in accordance with the structure of the substituent group. The hydrogen atom present in the group formyl, –CHO, is substitutable under the same conditions as those described in P-65.1.8.2 for formic acid.

Examples:

Cl-CO–
carbonochloridoyl (preferred prefix)
(not chloroformyl)

Br-CS–
carbonobromidothioyl (preferred prefix)
[not bromo(thioformyl)]

HCO-O–
formyloxy (preferred prefix)

HCO-S–
formylsulfanyl (preferred prefix)

P-65.2 CARBONIC, CYANIC, AND DI- AND POLYCARBONIC ACIDS

Carbonic acid, cyanic acid, and di- and polycarbonic acids are a group of functional parent compounds different from carboxylic acids; these acids have no hydrogen atom(s) to be used in substitutive nomenclature.

The following acids, classified as mononuclear carbon acids, have retained names that are preferred IUPAC names:

carbonic acid (PIN) HO-CO-OH

cyanic acid (PIN) HO-CN

The following di- or polynuclear carbon acids have retained names that are preferred IUPAC names:

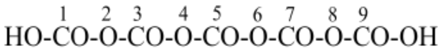
dicarbonic acid (PIN) HO-CO-O-CO-OH

tricarbonic acid (PIN) HO-CO-O-CO-O-CO-OH

tetracarbonic acid (PIN) HO-CO-O-CO-O-CO-O-CO-OH

polycarbonic acids HO-[CO-O]$_n$-H n = 5, 6 and higher homologues
are named by skeletal replacement (‘a’) nomenclature

Example:



$$\mathrm{HO\text{-}\overset{1}{C}O\text{-}\overset{2}{O}\text{-}\overset{3}{C}O\text{-}\overset{4}{O}\text{-}\overset{5}{C}O\text{-}\overset{6}{O}\text{-}\overset{7}{C}O\text{-}\overset{8}{O}\text{-}\overset{9}{C}O\text{-}OH}$$

3,5,7-trioxo-2,4,6,8-tetraoxanonanedioic acid (PIN)

The decreasing order of seniority of the carbon acids as indicated in Section P-41 is: polycarbonic acids > tetracarbonic acid > tricarbonic acid > dicarbonic acid > carbonic acid > cyanic acid.

P-65.2.1 Carbonic acid
P-65.2.2 Cyanic acid
P-65.2.3 Di-, tri-, tetra-, and polycarbonic acids

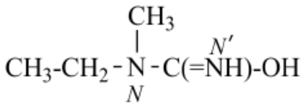
P-65.2.1 Carbonic acid

The nomenclature of chalcogen analogues and derivatives of carbonic acid is based on functional replacement of one oxygen in –OH groups or of the doubly bonded oxygen atom, =O, and is indicated by infixes. Substitution of formic acid is not recommended for generation of these names.

P-65.2.1.1 The contracted name ‘carbamic acid’ (from carbonamidic acid), for $H_2N\text{-}CO\text{-}OH$, and ‘carbamimidic acid’ (from carbonamidimidic acid), for $H_2N\text{-}C(=NH)\text{-}OH$, are retained and are the preferred IUPAC names.

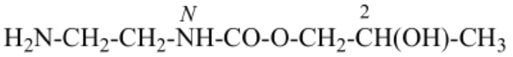
Examples:

$(CH_3)_2N\text{-}COOH$
dimethylcarbamic acid (PIN)



$$\mathrm{CH_3\text{-}CH_2\text{-}\underset{\mathit{N}}{\overset{\overset{\textstyle CH_3}{|}}{N}}\text{-}C(=\overset{\mathit{N'}}{N}H)\text{-}OH}$$

N-ethyl-*N*-methylcarbamimidic acid (PIN)



$$\mathrm{H_2N\text{-}CH_2\text{-}CH_2\text{-}\overset{\mathit{N}}{N}H\text{-}CO\text{-}O\text{-}CH_2\text{-}\overset{2}{C}H(OH)\text{-}CH_3}$$

2-hydroxypropyl (2-aminoethyl)carbamate (PIN)

P-65.2.1.2 Functional replacement in carbonic acid and carbamic acid names by –OO–, –S–, –Se–, and –Te– is expressed by the infixes ‘peroxo’, ‘thio’, ‘seleno’, and ‘telluro’, respectively. Tautomeric groups in mixed chalcocarbonic acids, such as HO-CO-SH or HO-CS-OH, are distinguished by prefixing italic element symbols, such as ‘*S*’ or ‘*O*’, respectively, to the term ‘acid’; the italic symbols ‘*OS*’ and ‘*SO*’ are used for peroxy acids.

Contrary to Rules P-65.1.3 through P-65.1.5, functional replacement nomenclature is applied to the retained name ‘carbamic acid’ and not to the systematic name ‘carbonamidic acid’.

Examples:

$H_2N\text{-}CS\text{-}OH$
carbamothioic *O*-acid (PIN)

$H_2N\text{-}CO\text{-}SeH$
carbamoselenoic *Se*-acid (PIN)

HO-CO-SH
carbonothioic *S*-acid (PIN)
(not sulfanylformic acid)

HSe-CO-SeH
carbonodiselenoic *Se,Se*-acid (PIN)

HS-CS-SH
carbonotrithioic acid (PIN)

$H_2N\text{-}CO\text{-}OOH$
carbamoperoxoic acid (PIN)

HO-CO-OOH
carbonoperoxoic acid (PIN)

HOO-CO-OOH
carbonodiperoxoic acid (PIN)

HO-CO-OSH
carbono(thioperoxoic) *OS*-acid (PIN)

HOS-CO-OSH
carbonobis(thioperoxoic) *OS*,*SO*-acid (PIN)

P-65.2.1.3 Functional replacement of =O in ‘carbonic acid’ and ‘carbamic acid’ by =NH and $=N\text{-}NH_2$ is expressed by the infixes ‘imido’ and ‘hydrazono’ and of oxygen in –OH groups in the resulting acids by chalcogen atoms is expressed by infixes, as in P-65.2.1.2. As described in P-65.2.1.1, the name ‘carbamimidic acid’ is retained for $H_2N\text{-}C(=NH)\text{-}OH$ (in place of the systematic name ‘carbonamidimidic acid’) and used as a preferred IUPAC name. It is modified by chalcogen atoms in functional replacement nomenclature in the same way as ‘carbamic acid’.

Italic letter locants *N*, *N′* etc. are used to designate substitution on nitrogen atoms.

Examples:

HO-C(=NH)-OH
carbonimidic acid (PIN)

$H_2N\text{-}C(=NH)\text{-}OH$
carbamimidic acid (PIN; retained name)

$HO\text{-}C(=N\text{-}NH_2)\text{-}OH$
carbonohydrazonic acid (PIN)

HS-C(=NH)-OH
carbonimidothioic acid (PIN)

$H_2N\text{-}C(=NH)\text{-}SH$
carbamimidothioic acid (PIN)

$HSe\text{-}C(=N\text{-}NH_2)\text{-}SeH$
carbonohydrazonodiselenoic acid (PIN)

$H_2N\text{-}C(=NH)\text{-}OSH$
carbamimido(thioperoxoic) *OS*-acid (PIN)

P-65.2.1.4 Functional replacement of one of the –OH groups of carbonic acid by various atoms or groups is expressed by the following infixes: fluorido, –F; chlorido, –Cl; bromido, –Br; iodido, –I; azido, $–N_3$; amido, $–NH_2$; cyanido, –CN; isocyanido, –NC; isocyanatido, –NCO; isothiocyanatido, –NCS; isoselenocyanatido, –NCSe; isotellurocyanatido, –NCTe (see P-67.1.2.3.2).

Italic letter locants *N*, *N′*, etc. are used to designate substitution on nitrogen atoms.

Replacement by the $–NHNH_2$ group results in hydrazinecarboxylic acid and related derivatives (see P-68.3.1.2).

Examples:

$H_2N\text{-}CO\text{-}OH$
carbamic acid (PIN; retained name)
(not carbonamidic acid)

H_2N-C(=NH)-OH
carbamimidic acid (PIN; retained name)
(not carbonamidimidic acid)

H_2N-CO-SH
carbamothioic *S*-acid (PIN)

H_2N-C(=NH)-SeH
carbamimidoselenoic acid (PIN)

Cl-CO-OH
carbonochloridic acid (PIN)

NC-CO-OH
carbonocyanidic acid (PIN)

N_3-CO-OH
carbonazidic acid (PIN)

SCN-CO-OH
carbonisothiocyanatidic acid (PIN)

H_2N-NH-CO-OH
hydrazinecarboxylic acid (PIN)
carbonohydrazidic acid
(carboxylic acids expressed by suffixes are preferred to carbonic acid analogues;
see P-41 and P-68.3.1.2.1)

P-65.2.1.5 Acyl groups derived from carbonic and related acids

Acyl groups derived from carbonic and related acids, including functional replacement analogues, by the removal of one or two hydroxy groups from the acid are named in accordance with the methodology described in P-65.1.7.2. Names are formed in two ways:

(1) Names may be formed by changing the -ic or -oic acid ending of the name of the acid to -yl or -oyl, respectively. Names of acyl groups ending in -yl are exceptions to the general rule (see P-65.1.7.2). This method is the traditional method that consists in removing the two hydroxy groups from carbonic acid or its analogues; it is now recommended to be used also when only one hydroxy group is present in an acid. It is also recommended that divalent acyl groups, such as 'carbonyl' represent only the 'diyl' type of substituent prefix in which the two free valences are divergent (symbols CO< or –CO–). Substituent prefixes in which both free valences are attached to the same atom are named by substitutive nomenclature, for example, =CO is named oxomethylidene (see P-65.2.1.8);

(2) Names may be formed by a concatenation operation, i.e., by adding appropriate monovalent substituent groups to divalent acyl groups such as 'carbonyl', 'carbonothioyl', and 'carbonimidoyl' formed by method (1).

Names formed by method (1) are preferred IUPAC names; they are preferred to other names for acyl groups, including the use of prefixes rather than infixes or names formed by full or partial concatenation.

Examples:

HO-CO-OH carbonic acid (PIN)	–CO– carbonyl (preferred prefix)
HO-CS-OH carbonothioic *O*,*O*-acid (PIN)	–CS– carbonothioyl (preferred prefix) thiocarbonyl
HO-C(=NH)-OH carbonimidic acid (PIN)	–C(=NH)– carbonimidoyl (preferred prefix)
HO-C(=NNH_2)-OH carbonohydrazonic acid (PIN)	–C(=N-NH_2)– carbonohydrazonoyl (preferred prefix)
H_2N-CO-OH carbamic acid (PIN)	H_2N-CO– carbamoyl (retained name; preferred prefix) aminocarbonyl
H_2N-CS-OH carbamothioic *O*-acid (PIN)	H_2N-CS– carbamothioyl (retained name; preferred prefix) aminocarbonothioyl
H_2N-C(=NH)-OH	H_2N-C(=NH)– carbamimidoyl– (retained name; preferred prefix)

carbamimidic acid (PIN)	*C*-aminocarbonimidoyl
Cl-CO-OH carbonochloridic acid (PIN)	Cl-CO– carbonochloridoyl (preferred prefix) chlorocarbonyl
NC-CO-OH carbonocyanidic acid (PIN)	NC-CO– carbonocyanidoyl (preferred prefix) cyanocarbonyl
Br-CS-OH carbonobromidothioic *O*-acid (PIN)	Br-CS– carbonobromidothioyl (preferred prefix) bromocarbonothioyl
Cl-C(=NH)-OH carbonochloridimidic acid (PIN)	Cl-C(=NH)– carbonochloridimidoyl (preferred prefix) *C*-chlorocarbonimidoyl
HOO-CO-OH carbonoperoxoic acid (PIN)	HOO-CO– carbonoperoxoyl (preferred prefix) hydroperoxycarbonyl

P-65.2.1.6 The prefix ‘carboxy’ and prefixes for chalcogen analogues.

The prefix ‘carboxy’ for –COOH is a retained prefix. Chalcogen analogues are named by functional replacement nomenclature provided that it is not necessary to specify the location of the chalcogen atom. Specification of chalcogen atoms is accomplished by compound prefixes formed by concatenation.

Examples:

–COSH or –CSOH
thiocarboxy (preferred prefix)

HS-CO–
sulfanylcarbonyl (preferred prefix)

HS-CS–
dithiocarboxy (preferred prefix)
sulfanylcarbonothioyl

HO-CS–
hydroxycarbonothioyl (preferred prefix)

HOOC-O–
carboxyoxy (preferred prefix)

HOOC-S–
carboxysulfanyl (preferred prefix)

HOOC-NH–
carboxyamino (preferred prefix)

HS-CO-O–
(sulfanylcarbonyl)oxy (preferred prefix)

P-65.2.1.7 Chalcogen analogues of the ‘carbonoperoxoyl’ prefix, –CO-OOH, are named in three ways:

(1) by using an infix when the position of the chalcogen atoms is not known;

(2) by compound prefixes formed by concatenation;

(3) by thiohydroperoxy prefixes using the italic prefixes *SO*- or *OS*-, as necessary.

Methods (1) or (2) lead to preferred IUPAC names.

Examples:

HOS-CSe–
(2) (hydroxysulfanyl)carbonoselenoyl (preferred prefix)
(3) (*OS*-thiohydroperoxy)carboselenoyl

HOS-CO– or HSO-CO–
(1) carbono(thioperoxoyl) (preferred prefix)
(3) (thiohydroperoxy)carbonyl

HS-O-CO-O–
(2) [(sulfanyloxy)carbonyl]oxy (preferred prefix)
(3) [(*SO*-thiohydroperoxy)carbonyl]oxy

HSS-CO-O–
(2) (disulfanylcarbonyl)oxy (preferred prefix)
(3) [(dithiohydroperoxy)carbonyl]oxy

P-65.2.1.8 Names of nonacyl substituent groups derived from carbonic acid

Acyl groups derived from carbonic acid and carbonic acids modified by functional replacement are divalent groups with the two free valences belonging to the 'diyl' type, such as CO<. When the two free valences are of the 'ylidene' type, =C=O for example, names of acyl groups are no longer used to designate such groups; systematic substitutive names are used instead.

Examples:

=C=O
oxomethylidene (preferred prefix)

=C=S
sulfanylidenemethylidene (preferred prefix)
thioxomethylidene

=C=NH
iminomethylidene (preferred prefix)

$=C=N-NH_2$
hydrazinylidenemethylidene (preferred prefix)
diazanylidenemethylidene

P-65.2.2 Cyanic acid

Cyanic acid is the retained name for NC-OH. The functional replacement name based on carbonic acid would be carbononitridic acid, but this name has not been used and, although systematic, is only recommended for general nomenclature. Cyanic acid is classified as an acid, thus generating anhydrides (see P-65.7.2) and esters (see P-65.6.3.2).

Preferred prefixes derived from cyanic acid are 'cyano' for –CN and 'cyanato' for –O-CN, 'thiocyanato' for –S-CN, 'selenocyanato' for –Se-CN, and 'tellurocyanato' for –Te-CN. Functional replacement by –OO–, –S–, –Se–, and –Te– is expressed by the appropriate functional replacement prefix. This exception to the use of infixes in the functional replacement nomenclature applied to the mononuclear inorganic acids (see P-67) is necessary to maintain well entrenched traditional names and their related isocyanates, such as isothiocyanates. Parentheses are used to enclose chalcogen prefixes to avoid the possibility of ambiguity.

Examples:

NC-SH thiocyanic acid (PIN) carbononitridothioic acid	NC-S– thiocyanato (preferred prefix) carbononitridoylsulfanyl carbononitridoylthio
NC-OOH peroxycyanic acid (PIN) carbononitridoperoxoic acid	NC-OO– cyanoperoxy (preferred prefix) carbononitridoylperoxy
NC-SS-H dithioperoxycyanic acid (PIN) carbononitrido(dithioperoxoic) acid	NC-SS– cyanodisulfanyl (preferred prefix) carbononitridoyldisulfanyl carbononitridoyldithio
$NC-CH_2-COOH$ cyanoacetic acid (PIN) carbononitridoylacetic acid	$NC-S-CH_2-CH_2-COOH$ 3-(thiocyanato)propanoic acid (PIN) 3-(carbononitridothio)propanoic acid

P-65.2.3 Di-, tri-, tetra-, and polycarbonic acids

Di-, tri-, tetra-, and polycarbonic acids belong to the series of homopolynuclear acids, whose central atom is carbon. Their generic formula is HO-[CO-O]$_n$-H, where *n* is 2, 3, 4, etc. and they are named by adding a multiplying prefix corresponding to the number of carbon atoms to the name of ‘carbonic acid’ or a functional replacement derivative. The structure is numbered consecutively from one end to the other, starting from and ending at a carbon atom:

Examples:

$$\text{HO-}\overset{1}{\text{C}}\text{O-}\overset{2}{\text{O}}\text{-}\overset{3}{\text{C}}\text{O-OH}$$

dicarbonic acid (PIN)

$$\text{HO-}\overset{1}{\text{C}}\text{O-}\overset{2}{\text{O}}\text{-}\overset{3}{\text{C}}\text{O-}\overset{4}{\text{O}}\text{-}\overset{5}{\text{C}}\text{O-OH}$$

tricarbonic acid (PIN)

P-65.2.3.1 Functional replacement for di-, tri-, tetra-, and polynuclear carbon acids

P-65.2.3.1.1 General methodology
P-65.2.3.1.2 Replacement by –OO–, –S–, =S, –Se–, =Se, –Te–, =Te, –NH–, =NH, and $=NHNH_2$
P-65.2.3.1.3 Replacement by halides and pseudohalides
P-65.2.3.1.4 Replacement by $–NH_2$ and $–NHNH_2$ groups.
P-65.2.3.1.5 Substituent groups derived from di-, tri-, tetra-, and polycarboic acids

P-65.2.3.1.1 General methodology

Nomenclature for functional analogues of the di-, tri-, tetra-, and polycarbonic acids follows the principles for naming polynuclear inorganic oxo acids (see P-67.2.1). Prefixes are used to indicate functional replacement and the chain is numbered consecutively from one end to the other, starting from and ending at a carbon atom. These prefixes are listed in Table 4.2; they are cited in alphabetical order in front of the retained name of the polyacid, with appropriate locants as required.

P-65.2.3.1.2 Replacement by –OO–, –S–, =S, –Se–, =Se, –Te–, =Te, –NH–, =NH, and $=NHNH_2$

Functional replacement of oxygen atom(s), –OH, =O, –O–, is denoted by prefixes, i.e., peroxy for –OO–; thio for –S– or =S; seleno for –Se– or =Se; telluro for –Te–or =Te; imido for –NH– or =NH, and hydrazono for $=NHNH_2$. The position of each replaced oxygen atom is denoted by the appropriate numerical locant.

P-65.2.3.1.2.1 Superscripted italic letter locants N^2, N^3, etc. are used to designate substitution on nitrogen atoms that are not amide linkages that are part of the chain for which arabic numbers are used as locants.

> This is a change. Primed letter locants, *N*′, *N*″, *N*‴, etc. were previously used as locants for nitrogen atoms that are not amide linkages that are part of the chain for which arabic numbers are used as locants.

Examples:

$$\text{HO-}\overset{1}{\text{C}}\text{O-}\overset{2}{\text{S}}\text{-}\overset{3}{\text{C}}\text{O-OH}$$

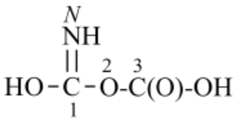
2-thiodicarbonic acid (PIN)

$$\text{HO-}\overset{1}{\text{C}}\text{O-}\overset{2}{\text{NH}}\text{-}\overset{3}{\text{C}}\text{O-OH}$$

2-imidodicarbonic acid (PIN)

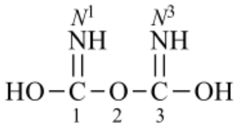
$$\text{HO-}\overset{1}{\text{C}}\text{O-}\overset{2}{\text{OO}}\text{-}\overset{3}{\text{C}}\text{O-OH}$$

2-peroxydicarbonic acid (PIN)



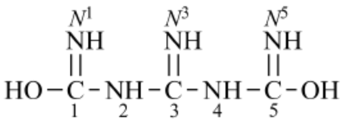
$$\text{HO}-\underset{1}{\overset{\overset{N}{\text{NH}}}{\overset{\|}{\text{C}}}}-\overset{2}{\text{O}}\text{-}\overset{3}{\text{C}}\text{(O)-OH}$$

1-imidodicarbonic acid (PIN)



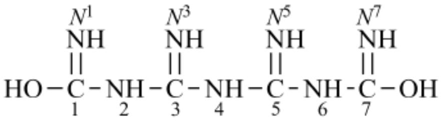
$$\text{HO}-\underset{1}{\overset{\overset{N^1}{\text{NH}}}{\overset{\|}{\text{C}}}}-\underset{2}{\text{O}}-\underset{3}{\overset{\overset{N^3}{\text{NH}}}{\overset{\|}{\text{C}}}}-\text{OH}$$

1,3-diimidodicarbonic acid (PIN)



$$\text{HO}-\underset{1}{\overset{\overset{N^1}{\text{NH}}}{\overset{\|}{\text{C}}}}-\underset{2}{\text{NH}}-\underset{3}{\overset{\overset{N^3}{\text{NH}}}{\overset{\|}{\text{C}}}}-\underset{4}{\text{NH}}-\underset{5}{\overset{\overset{N^5}{\text{NH}}}{\overset{\|}{\text{C}}}}-\text{OH}$$

1,2,3,4,5-pentaimidotricarbonic acid (PIN)



$$\text{HO}-\underset{1}{\overset{\overset{N^1}{\text{NH}}}{\overset{\|}{\text{C}}}}-\underset{2}{\text{NH}}-\underset{3}{\overset{\overset{N^3}{\text{NH}}}{\overset{\|}{\text{C}}}}-\underset{4}{\text{NH}}-\underset{5}{\overset{\overset{N^5}{\text{NH}}}{\overset{\|}{\text{C}}}}-\underset{6}{\text{NH}}-\underset{7}{\overset{\overset{N^7}{\text{NH}}}{\overset{\|}{\text{C}}}}-\text{OH}$$

1,2,3,4,5,6,7-heptaimidotetracarbonic acid (PIN)

$$\text{HO-}\overset{3}{\text{C}}\text{O-}\overset{2}{\text{O}}\text{-}\overset{1}{\text{C}}\text{O-OOH}$$

1-peroxydicarbonic acid (PIN)

$$\text{HOO-}\overset{1}{\text{C}}\text{O-}\overset{2}{\text{O}}\text{-}\overset{3}{\text{C}}\text{O-OOH}$$

1,3-diperoxydicarbonic acid (PIN)

P-65.2.3.1.2.2 When necessary, letter locants *O*, *S*, *Se*, and *Te* are used, as appropriate, to designate the position of a chalcogen atom replacing oxygen in –OH or =O groups. Superscripted letter locants, such as O^x, S^x, Se^x, and Te^x, are placed before the term 'acid' as needed.

The use of superscripted letter locants is a change from previous practice where numerical locants were placed in front of the letter locants such as 1-*O* and 3-*O*, as described in ref. 1, Rule C-213.1.

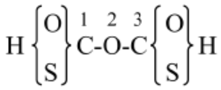
Examples:

$$\text{HS-}\overset{3}{\text{C}}\text{S-}\overset{2}{\text{O}}\text{-}\overset{1}{\text{C}}\text{S-SH}$$

1,1,3,3-tetrathiodicarbonic acid (PIN)

$$\text{HS-}\overset{1}{\text{C}}\text{S-}\overset{2}{\text{S}}\text{-}\overset{3}{\text{C}}\text{S-SH}$$

pentathiodicarbonic acid (PIN)



$$\text{H}\left\{\begin{matrix}\text{O}\\ \text{S}\end{matrix}\right\}\overset{1}{\text{C}}\text{-}\overset{2}{\text{O}}\text{-}\overset{3}{\text{C}}\left\{\begin{matrix}\text{O}\\ \text{S}\end{matrix}\right\}\text{H}$$

1,3-dithiodicarbonic acid (PIN;
the location of the sulfur atoms is unknown)

$$\text{HS-}\overset{1}{\text{C}}\text{O-}\overset{2}{\text{O}}\text{-}\overset{3}{\text{C}}\text{O-SH}$$

1,3-dithiodicarbonic S^1,S^3-acid (PIN)

$$\text{HO-}\overset{1}{\text{C}}\text{S-}\overset{2}{\text{O}}\text{-}\overset{3}{\text{C}}\text{S-OH}$$

1,3-dithiodicarbonic O^1,O^3-acid (PIN)

P-65.2.3.1.2.3 Compound substituent groups may have to be used to name chalcogen analogues when the location of chalcogen atoms is not known.

Examples:

H{S/O}C-O-CO-SH [(thiocarboxy)oxy]methanethioic *S*-acid (PIN)

H{S/O}C-O-CS-OH [(thiocarboxy)oxy]methanethioic *O*-acid (PIN)

P-65.2.3.1.3 Replacement by halides and pseudohalides

Prefixes bromo for –Br, chloro for –Cl, fluoro for –F, iodo for –I , azido for $-N_3$, isocyano for –NC, and isocyanato for –NCO (and chalcogen analogues) are used to indicate functional replacement.

Examples:

$$\text{Cl-}\overset{1}{\text{C}}\text{O-}\overset{2}{\text{O}}\text{-}\overset{3}{\text{C}}\text{O-OH}$$

chlorodicarbonic acid (PIN)

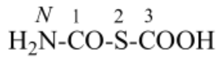
$$\text{OCN-}\overset{1}{\text{C}}\text{O-}\overset{2}{\text{N}}\text{H-}\overset{3}{\text{C}}\text{O-OH}$$

2-imido-1-isocyanatodicarbonic acid
(locants are used to avoid ambiguity)

P-65.2.3.1.4 Replacement by NH_2 and $NHNH_2$ groups

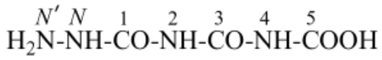
The prefixes amido and hydrazido are used to indicate functional replacement by $-NH_2$ and $-NHNH_2$ groups, respectively. Italic letter locants *N*, *N*′, etc. are used to designate substitution on nitrogen atoms that are not amide linkages for which numerical locants are used.

Examples:



$H_2\overset{N}{N}\text{-}\overset{1}{C}O\text{-}\overset{2}{S}\text{-}\overset{3}{C}OOH$

1-amido-2-thiodicarbonic acid (PIN)



$H_2\overset{N'}{N}\text{-}\overset{N}{N}H\text{-}\overset{1}{C}O\text{-}\overset{2}{N}H\text{-}\overset{3}{C}O\text{-}\overset{4}{N}H\text{-}\overset{5}{C}OOH$

1-hydrazido-2,4-diimidotricarbonic acid (PIN)

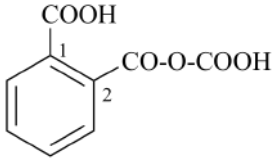
P-65.2.3.1.5 Substituent groups derived from di-, tri-, tetra-, and polycarbonic acids

Names of substituent groups are formed by substitution or concatenation as required.

Examples:

HOOC-O-CO–
(carboxyoxy)carbonyl (preferred prefix)
[not (carboxyoxy)formyl]

HS-CS-S-CS–
[(dithiocarboxy)sulfanyl]carbonothioyl (preferred prefix)
[(sulfanylcarbonothioyl)sulfanyl]carbonothioyl
[sulfanyl(thiocarbonyl)sulfanyl](thiocarbonyl)
{not [(dithiocarboxy)sulfanyl]thioformyl}



2-[(carboxyoxy)carbonyl]benzoic acid (PIN)

P-65.3 SULFUR, SELENIUM, AND TELLURIUM ACIDS WITH CHALCOGEN ATOMS DIRECTLY LINKED TO A PARENT HYDRIDE

P-65.3.0 Introduction. The following acids are included in this section:

$R\text{-}SO_3H$ sulfonic acids

$R\text{-}SeO_3H$ selenonic acids

$R\text{-}TeO_3H$ telluronic acids

$R\text{-}SO_2H$ sulfinic acids

$R\text{-}SeO_2H$ seleninic acids

$R\text{-}TeO_2H$ tellurinic acids

Table 6.2 Suffixes and prefixes used to denote sulfur, selenium, and tellurium acids with chalcogen atoms directly linked to a parent

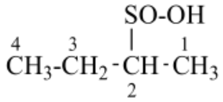
Group	Preselected Suffix	Preselected Prefix
$-SO_2\text{-}OH$	sulfonic acid	sulfo
$-S(O)\text{-}OH$	sulfinic acid	sulfino
$-SeO_2\text{-}OH$	selenonic acid	selenono
$-Se(O)\text{-}OH$	seleninic acid	selenino
$-TeO_2\text{-}OH$	telluronic acid	tellurono
$-Te(O)\text{-}OH$	tellurinic acid	tellurino

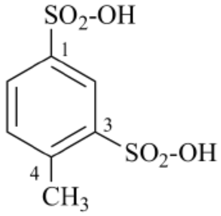
P-65.3.1 Substitutive nomenclature, suffix mode, for sulfonic, sulfinic, etc., acids

Sulfonic, sulfinic, etc., acids are named substitutively by adding an appropriate suffix listed in Table 6.2 to the name of a parent hydride name. Multiplying prefixes ‘di’, ‘tri’, ‘tetra’, etc. are used to denote multiplicity of suffixes. The name ‘sulfanilic acid’ is not retained.

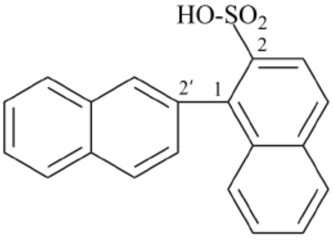
Examples:

C_6H_5-SO_2-OH
benzenesulfonic acid (PIN)

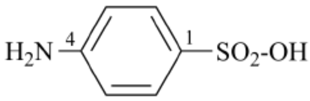

$$\overset{4}{C}H_3\text{-}\overset{3}{C}H_2\text{-}\underset{2}{\overset{SO\text{-}OH}{CH}}\text{-}\overset{1}{C}H_3$$
butane-2-sulfinic acid (PIN)



4-methylbenzene-1,3-disulfonic acid (PIN)
(not toluene-2,4-disulfonic acid)



[1,2′-binaphthalene]-2-sulfonic acid (PIN)



4-aminobenzene-1-sulfonic acid (PIN)
(not ‘sulfanilic acid’; this name is not retained)

P-65.3.1.1 Modification by functional replacement

Oxygen atoms of a suffix acid may be replaced by –OO– and/or other chalcogen analogues, –S– or =S, –Se– or =Se, –Te– or =Te, =NH, and =N-NH_2 by functional replacement nomenclature. The general methodology is to modify the suffixes by infixes and use them in systematic substitutive nomenclature in the way prescribed for unmodified suffixes. If necessary, names are formed in accordance with the order of seniority, unmodified acids followed by –OO– > S > Se > Te. This seniority is fully exemplified in Section P-43.

P-65.3.1.2 Peroxy acids

The suffixes given in Table 6.2 are modified by the infix ‘peroxo’ for use in substitutive nomenclature as illustrated by the following suffixes.

–SO_2-OOH
sulfonoperoxoic acid (preferred suffix)

–SeO-OOH
seleninoperoxoic acid (preferred suffix)

Examples:

CH_3-SO_2-OOH
methanesulfonoperoxoic acid (PIN)

C_6H_5-TeO-OOH
benzenetellurinoperoxoic acid (PIN)

P-65.3.1.3 Modification by other chalcogen atoms

Suffixes are modified by the infixes ‘thio’, for –S– or =S, ‘seleno’, for –Se– or =Se, and ‘telluro’, for –Te– or =Te, and used as such. Tautomers are denoted by symbols *S*, *Se*, and *Te* placed in front of the term ‘acid’, to express positions of chalcogen atoms when known. The infixes ‘thioperoxo’, ‘selenoperoxo’, etc. are used to indicate functional replacement in peroxy acids.

–SO_2-SH
sulfonothioic *S*-acid (preselected suffix)

–Se(=S)-OH
seleninothioic *O*-acid (preselected suffix)

$–SO_2\text{-}OSH$
sulfono(thioperoxoic) *OS*-acid (preselected suffix)

–TeO-SeSH
tellurino(selenothioperoxoic) *SeS*-acid (preselected suffix)

Examples:

$CH_3\text{-}CH_2\text{-}CH_2\text{-}S\{O/Se\}H$
propane-1-sulfinoselenoic acid (PIN)

$CH_3\text{-}CH_2\text{-}S(O)(S)\text{-}OH$
ethanesulfonothioic *O*-acid (PIN)

$CH_3\text{-}CH_2\text{-}Se(=S)\text{-}OH$
ethaneseleninothioic *O*-acid (PIN)

P-65.3.1.4 Imidic and hydrazonic acids derived from sulfonic, sulfinic, etc. acids

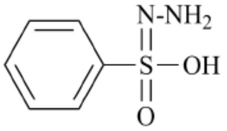
Imidic acids and hydrazonic acids derived from sulfonic, sulfinic, etc., acids are named by using suffixes such as 'sulfinimidic acid' for –S(=NH)-OH, 'sulfonohydrazonic acid' for $–S(O)(=NNH_2)\text{-}OH$. The prefix 'di' is used to indicate the replacement of two oxygen atoms (=O) in sulfonic acids, for example, 'sulfonodiimidic acid' for $–S(=NH)_2\text{-}OH$. Suffixes are listed in Table 4.3.

Examples:

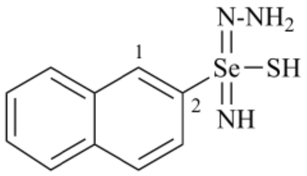
$CH_3\text{-}CH_2\text{-}S(=NH)_2\text{-}OH$
ethanesulfonodiimidic acid (PIN)

$CH_3\text{-}S(=NH)\text{-}OH$
methanesulfinimidic acid (PIN)

$C_6H_5\text{-}Se(=NH)_2\text{-}OH$
benzeneselenonodiimidic acid (PIN)



benzenesulfonohydrazonic acid (PIN)

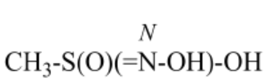


naphthalene-2-selenonohydrazonimidothioic acid (PIN)

P-65.3.1.5 Hydroximic and hydroxamic acids derived from sulfonic, sulfinic, etc. acids

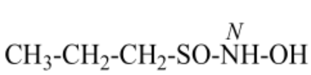
Hydroximic acids and hydroxamic acids derived from sulfonic, sulfinic, etc. acids are named as *N*-hydroxysulfonimidic acids and *N*-hydroxysulfonamides, etc. (see P-66.1.1.3.2), respectively.

Examples:



$CH_3\text{-}S(O)(=\overset{N}{N}\text{-}OH)\text{-}OH$

N-hydroxymethanesulfonimidic acid (PIN)



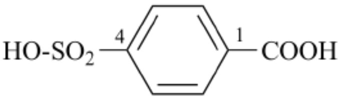
$CH_3\text{-}CH_2\text{-}CH_2\text{-}SO\text{-}\overset{N}{N}H\text{-}OH$

N-hydroxypropane-1-sulfinamide (PIN)

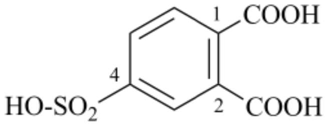
P-65.3.2 Substitutive nomenclature, prefix mode for sulfonic, sulfinic, etc. acids

P-65.3.2.1 When another group is also present that has seniority for citation as principal group (see P-41, P-42, P-43), or when all groups cannot be expressed as suffixes, organic oxoacids of sulfur, selenium or tellurium are named by adding to the name of the parent compound the appropriate prefix given in Table 6.2. These prefixes can be modified by prefixes designating chalcogen atoms in functional replacement nomenclature when the position of the chalcogen atom is not known or when it is not desirable to indicate such position.

Examples:



4-sulfobenzoic acid (PIN)



4-sulfobenzene-1,2-dicarboxylic acid (PIN)
4-sulfophthalic acid

$HO\text{-}SO_2\text{-}\overset{1}{C}H_2\text{-}\overset{2}{C}H_2\text{-}\overset{3}{C}H_2\text{-}\overset{4}{C}H_2\text{-}O\text{-}S\text{-}CH_2\text{-}O\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}SO_2\text{-}OH$

4-({[(3-sulfopropoxy)methyl]sulfanyl}oxy)butane-1-sulfonic acid (PIN)

$HO\text{-}SO\text{-}CH_2\text{-}COOH$

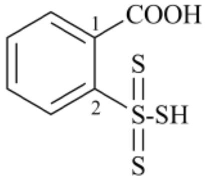
sulfinoacetic acid (PIN)

$HOO\overset{1}{C}\text{-}\overset{2}{C}H_2\text{-}\overset{3}{C}H_2\text{-}SeO_2\text{-}OH$

3-selenonopropanoic acid (PIN)

$H\{S/O\}S\text{-}CH_2\text{-}CH_2\text{-}SO_2\text{-}OH$

2-(thiosulfino)ethane-1-sulfonic acid



2-(trithiosulfo)benzoic acid (PIN)
2-(sulfanylsulfonodithioyl)benzoic acid

P-65.3.2.2 Acyl groups derived from sulfonic, sulfinic, etc. acids and their functional replacement analogues

P-65.3.2.2.1 Acyl sulfonic, sulfinic, selenonic, seleninic, telluronic, and tellurinic groups, $R\text{-}EO_x\text{–}$, $\text{–}O_xE\text{-}R\text{-}EO_x\text{–}$ or $\text{–}O_xE\text{-}R\text{-}[R'\text{-}EO_x\text{-}]\text{-}R''\text{-}EO_x\text{–}$, where E = S, Se, or Te, x = 1 or 2, and R, R′, and R″ are chains, rings, or ring systems; their functional replacement analogues are groups derived by the removal of the hydroxy group from each sulfonic, sulfinic, or related selenium or tellurium acid group that is expressed as the principal characteristic group by an appropriate suffix.

P-65.3.2.2.2 Names for acyl groups derived from sulfonic and sulfinic acids, and their Se and Te counterparts, by removal of the -OH group from each sulfonic, sulfinic, etc. acid expressed as a suffix are formed by changing the ‘ic acid’ ending of the suffix to ‘yl’. When the suffix is modified by functional replacement nomenclature, the ending of the corresponding acyl group is ‘oyl’. Acyl groups formed by concatenation, for example, phenylsulfonyl, may be used in general nomenclature.

The formation of simple substitutive preferred acyl prefixes directly from the name of the sulfonic acid, sulfinic acid, etc., as in ‘benzenesulfonyl’, instead of the traditional method of concatenation as in ‘phenylsulfonyl’ is a distinct change to simplify names. To facilitate name interpretation, the preferred prefixes are enclosed in parentheses even though they are simple prefixes (P-16.5.1.4).

Examples:

$C_6H_5\text{-}SO_2\text{–}$

benzenesulfonyl (preferred prefix)
phenylsulfonyl

$CH_3\text{-}Se(O)\text{–}$

methaneseleninyl (preferred prefix)
methylseleninyl

$CH_3\text{-}CH_2\text{-}S(O)(S)\text{–}$

ethanesulfonothioyl (preferred prefix)
ethylsulfonothioyl

C_6H_5-S(Se)–
benzenesulfinoselenoyl (preferred prefix)
phenylsulfinoselenoyl

CH_3-CH_2-S(=NH)–
ethanesulfinimidoyl (preferred prefix)
ethylsulfinimidoyl

P-65.3.2.3 Substituent groups formed by concatenation

When the name of an acyl group cannot be derived directly from that of the acid expressed by a suffix, a concatenation procedure is used. For this procedure names of divalent mononuclear acyl groups are required. Acyl groups corresponding to sulfuric and sulfurous acids and the corresponding selenium and tellurium acids are formed from the acids by subtracting all -OH groups from the parent acid. The names used in the nomenclature of organic compounds are as follows:

–SO_2–
sulfonyl (preselected prefix)
sulfuryl

–SO–
sulfinyl (preselected prefix)
thionyl

–SeO_2–
selenonyl (preselected prefix)

–SeO–
seleninyl (preselected prefix)

–TeO_2–
telluronyl (preselected prefix)

–TeO–
tellurinyl (preselected prefix)

These acyl groups are modified by infixes in functional replacement nomenclature to indicate replacement by '=S', '=Se', '=Te', '=NH', and '=N-NH_2'.

Examples:

–S(=O)(=S)–
sulfonothioyl (preselected prefix)

–S(=S)(=S)–
sulfonodithioyl (preselected prefix)

–S(=NH)–
sulfinimidoyl (preselected prefix)

–Se(=O)(=NNH_2)–
selenonohydrazonoyl (preselected prefix)

–Se(=S)(=NH)–
selenonimidothioyl (preselected prefix)

Prefixes denoting characteristic groups can then be attached to these divalent acyl group names. The prefix 'hydro-' for H can also be used. This traditional method generates preferred IUPAC names. Names of acyl groups derived directly from the names sulfuric acid and sulfurous acid, and their Se and Te congeners, are inappropriate because of ambiguity and incompleteness (see P-67.1.4.4.1). The name sulfamoyl for H_2N-SO_2– is a retained name used as a preferred IUPAC name

Examples:

CH_3O-SO_2–
methoxysulfonyl (preferred prefix)

Cl-S(O)–
chlorosulfinyl (preselected prefix)

$H_2N\text{-}SO_2\text{–}$
sulfamoyl (preselected prefix)
aminosulfonyl

H-SO–
hydrosulfinyl (preselected prefix)

$CH_3\text{-}CO\text{-}O\text{-}SO_2\text{–}$
(acetyloxy)sulfonyl (preferred prefix)
acetoxysulfonyl

$CH_3\text{-}O\text{-}S(=NH)\text{–}$
S-methoxysulfinimidoyl (preferred prefix)

$HO\text{-}SO_2\text{-}O\text{–}$
sulfooxy (preselected prefix)

$H\text{-}SeO_2\text{–}$
hydroselenonyl (preselected prefix)

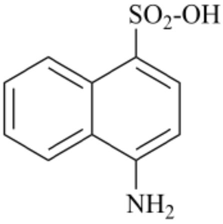
$\text{–}S\text{-}SO_2\text{-}S\text{–}$
sulfonylbis(sulfanediyl) (preselected prefix)

–O-SO-O–
sulfinobis(oxy) (preselected prefix)

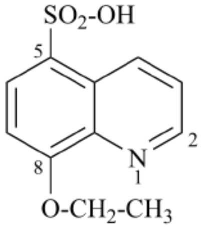
P-65.3.3 Polyfunctional compounds

Polyfunctional compounds are named in accordance with the general order of seniority of suffixes described in Sections P-41 and P-43. When required, numbering is based on the seniority order described in P-61.1.

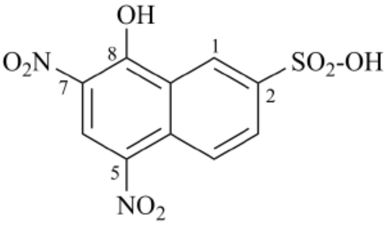
Examples:



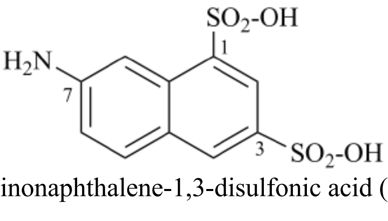
4-aminonaphthalene-1-sulfonic acid (PIN)



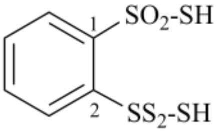
8-ethoxyquinoline-5-sulfonic acid (PIN)



8-hydroxy-5,7-dinitronaphthalene-2-sulfonic acid (PIN)



7-aminonaphthalene-1,3-disulfonic acid (PIN)



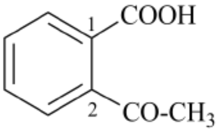
2-(trithiosulfo)benzene-1-sulfonothioic *S*-acid (PIN)

P-65.4 ACYL GROUPS AS SUBSTITUENT GROUPS

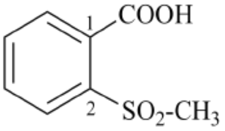
P-65.4.1 General methodology

Acyl group names that are described in preceding sections are used unchanged to denote substituent groups. Thus, the traditional way of using acyl groups derived from acyclic carboxylic acids to name ketones, pseudoketones, and heterones is maintained (see P-65.1.7 for more examples).

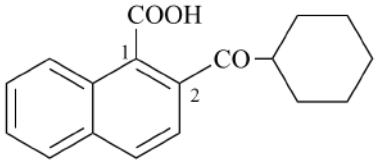
Examples:



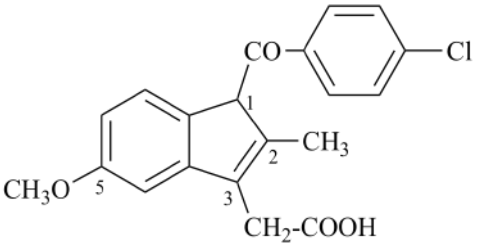
2-acetylbenzoic acid (PIN)



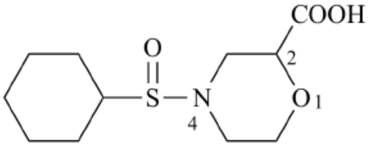
2-(methanesulfonyl)benzoic acid (PIN)
2-(methylsulfonyl)benzoic acid



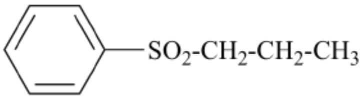
2-(cyclohexanecarbonyl)naphthalene-1-carboxylic acid (PIN)
2-(cyclohexylcarbonyl)naphthalene-1-carboxylic acid



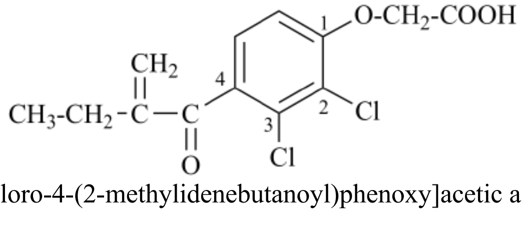
[1-(4-chlorobenzoyl)-5-methoxy-2-methyl-1*H*-inden-3-yl]acetic acid (PIN)



4-(cyclohexanesulfinyl)morpholine-2-carboxylic acid (PIN)
4-(cyclohexylsulfinyl)morpholine-2-carboxylic acid



(propane-1-sulfonyl)benzene (PIN)
(propylsulfonyl)benzene



[2,3-dichloro-4-(2-methylidenebutanoyl)phenoxy]acetic acid (PIN)

P-65.5 ACYL HALIDES AND PSEUDOHALIDES

P-65.5.1 Acyl halides from suffix acids
P-65.5.2 Acyl pseudohalides from suffix acids
P-65.5.3 Acyl halides and pseudohalides from carbonic, cyanic, and polycarbonic acids
P-65.5.4 Acyl halides and pseudohalides as substituent groups

P-65.5.1 Acyl halides from suffix acids

Acyl halides in which hydroxy groups of all acid groups expressed as the suffix denoting the principal characteristic group (carboxylic, sulfonic, sulfinic, selenonic, etc. acids) have been replaced by halogen atoms (F, Cl, Br, and I) are named by citing the name of the acyl group (see P-65.1.7) followed by the name(s) of the specific class(es) as a separate word(s), in alphabetical order, each preceded by a multiplicative prefix, as needed.

Table 6.3 Acyl halide and pseudohalide classes

	Halide	**Prefix**		**Pseudohalide**	**Prefix**
–F	fluoride	fluoro	$-N_3$	azide	azido
–Cl	chloride	chloro	–CN	cyanide	cyano
–Br	bromide	bromo	–NC	isocyanide	isocyano
–I	iodide	iodo	–NCO	isocyanate	isocyanato
			–NCS	isothiocyanate	isothiocyanato
			–NCSe	isoselenocyanate	isoselenocyanato
			–NCTe	isotellurocyanate	isotellurocyanato

The names formyl, acetyl, benzoyl, oxalyl, and oxamoyl are retained as preferred prefixes.

Examples:

$$\overset{2}{C}H_3\text{-}\overset{1}{C}O\text{-}Cl$$

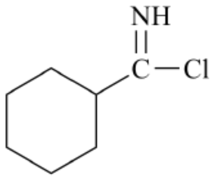
acetyl chloride (PIN)

HCO-Br

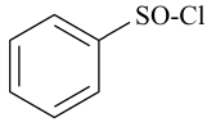
formyl bromide (PIN)

$$\overset{6}{C}H_3\text{-}\overset{5}{C}H_2\text{-}\overset{4}{C}H_2\text{-}\overset{3}{C}H_2\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}O\text{-}F$$

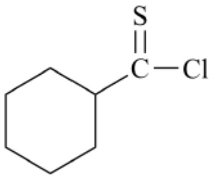
hexanoyl fluoride (PIN)



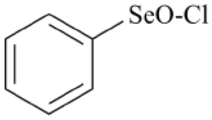
cyclohexanecarboximidoyl chloride (PIN)



benzenesulfinyl chloride (PIN)



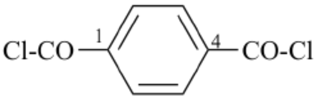
cyclohexanecarbothioyl chloride (PIN)



benzeneseleninyl chloride (PIN)

$Cl-CO-CH_2-CO-Cl$
propanedioyl dichloride (PIN)
malonyl dichloride

Cl-CO-CO-Cl
oxalyl dichloride (PIN)
ethanedioyl dichloride



benzene-1,4-dicarbonyl dichloride (PIN)
terephthaloyl dichloride

$Br-O_2S-CH_2-CH_2-SO_2-Br$
ethane-1,2-disulfonyl dibromide (PIN)

$Br-CO-CH_2-CH_2-CO-Cl$
butanedioyl bromide chloride (PIN)
succinyl bromide chloride

$H_2N-CO-CO-Br$
oxamoyl bromide (PIN)

P-65.5.2 Acyl pseudohalides from suffix acids

P-65.5.2.1 Acyl pseudohalides in which hydroxy groups of all acid groups expressed as the suffix denoting the principal characteristic group (carboxylic, sulfonic, sulfinic, selenonic, etc. acids) have been replaced by pseudohalogen groups (N_3, CN, NC, NCO, NCS, NCSe, NCTe) are named by citing the name of the acyl group (see P-65.1.7) followed by the name(s) of the class(es) as separate words, preceded by a multiplicative prefix, as needed. When a choice has to be made, the senior pseudohalide group is chosen in accordance with the decreasing order of seniority: N_3 > CN > NC > NCO > NCS > NCSe > NCTe. Halogen atoms are senior to pseudohalogen groups.

The names formyl, acetyl, benzoyl, oxalyl, and oxamoyl are retained to generate preferred IUPAC names.

Examples:

$\overset{4}{C}H_3-\overset{3}{C}H_2-\overset{2}{C}H_2-\overset{1}{C}O-CN$
butanoyl cyanide (PIN)
butyryl cyanide

SCN-CO-CO-NCS
oxalyl diisothiocyanate (PIN)

$CN-\overset{4}{C}O-\overset{3}{C}H_2-\overset{2}{C}H_2-\overset{1}{C}O-NCS$
butanedioyl isocyanide isothiocyanate (PIN)

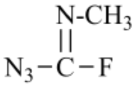
P-65.5.3 Acyl halides and pseudohalides from carbonic, cyanic, and polycarbonic acids

P-65.5.3.1 Acyl groups derived from carbonic acid, carbamic acid, and related acids, such as ‘carbonyl’ from carbonic acid, ‘carbamoyl’ from carbamic acid, and ‘carbamimidoyl’ from carbamimidic acid are used to form the names of the corresponding acyl halides.

Examples:

Cl-CO-Cl
carbonyl dichloride (PIN)

Br-CO-Cl
carbonyl bromide chloride (PIN)
(not carbonobromidic chloride)



$N_3\text{-}\overset{N\text{-}CH_3}{\overset{||}{C}}\text{-}F$

N-methylcarbonazidimidoyl fluoride (PIN)

NC-CO-Cl
carbonocyanidoyl chloride (PIN)

H_2N-CO-NCO
carbamoyl isocyanate (PIN)

P-65.5.3.2 As there is no acyl group derived from di- and polycarbonic acids, names for acyl halides derived from these acids are formed by using the name of the acid followed by the name(s) of the halides (see P-67.2.3 for the same methodology applied to inorganic polyacids).

Examples:

Cl-CO-O-CO-Cl
dicarbonic dichloride (PIN)

Cl-CO-O-CO-Br
dicarbonic bromide chloride (PIN)

$Cl\text{-}\overset{1}{C}O\text{-}\overset{2}{N}H\text{-}\overset{3}{C}O\text{-}Cl$
2-imidodicarbonic dichloride (PIN)

OCN-CO-O-CO-NCO
dicarbonic diisocyanate (PIN)

$Cl\text{-}\overset{1}{C}(=\overset{N}{N}H)\text{-}\overset{2}{N}H\text{-}\overset{3}{C}O\text{-}\overset{4}{S}\text{-}\overset{5}{C}(S)\text{-}Br$
1,2-diimido-4,5-dithiotricarbonic 5-bromide 1-chloride (PIN)

P-65.5.3.3 Acyl halides and pseudohalides from cyanic acid are formed in two ways:

(1) as acyl halides or pseudohalides of carbononitridic acid;

(2) by citing the name of the halide or pseudohalide after the name of the acid.

Method (1) generates preferred IUPAC names.

Examples:

NC-Cl
carbononitridic chloride (PIN)
cyanic chloride

$NC\text{-}N_3$
carbononitridic azide (PIN)
cyanic azide

P-65.5.4 Acyl halides and pseudohalides as substituent groups

When another group is present that has priority for citation as principal group or when attached to another substituting group, an acyl halide or pseudohalide is expressed:

(1) by a prefix formed from the name of the acid, for example, 'carbonochloridoyl';

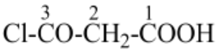
(2) by a compound prefix composed of a halo or halogeno prefix and an appropriate divalent acyl group, such as 'sulfonyl', for example, fluorosulfonyl;

(3) at the end of an acyclic carbon chain by a prefix denoting the halide or pseudohalide group and the prefix 'oxo', or a chalcogen analogue of oxo, such as sulfanylidene.

Method (1) leads to preferred IUPAC names when the suffix '-carboxylic acid' is used to name the corresponding acid; method (3) generates preferred IUPAC names for acyclic carbon chains.

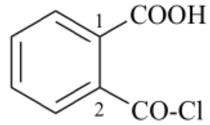
Seniority for numbering follows that for acids, for which see P-65.1.2.3. For seniority of halides and pseudohalides, see P-65.5.2.1.

Examples:

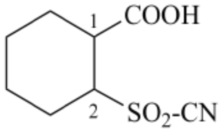


$\overset{3}{C}l\text{-}\overset{}{CO}\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}OOH$

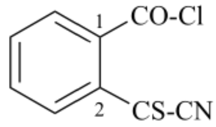
(3) 3-chloro-3-oxopropanoic acid (PIN)
(1) carbonochloridoylacetic acid



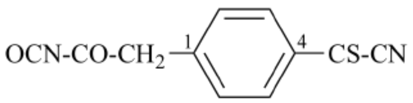
(1) 2-carbonochloridoylbenzoic acid (PIN)
(2) 2-(chlorocarbonyl)benzoic acid



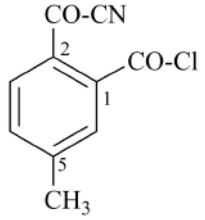
(1) 2-(cyanosulfonyl)cyclohexane-1-carboxylic acid (PIN)
(2) 2-sulfurocyanidoylcyclohexane-1-carboxylic acid



(1) 2-carbonocyanidothioylbenzoyl chloride (PIN)
(2) 2-(cyanocarbonothioyl)benzoyl chloride



(4-carbonocyanidothioylphenyl)acetyl isocyanate (PIN)
[not 4-(2-isocyanato-2-oxoethyl)benzenecarbothioyl cyanide,
acetyl is senior to carbothioyl]



2-carbonocyanidoyl-5-methylbenzoyl chloride (PIN)
2-(cyanocarbonyl)-5-methylbenzoyl chloride

$Br\text{-}CO\text{-}CO\text{-}CH_2\text{-}COOH$
(3) 4-bromo-3,4-dioxobutanoic acid (PIN)

$Br\text{-}CO\text{-}O\text{-}CO\text{-}CH_2\text{-}COOH$
(1) 3-(carbonobromidoyloxy)-3-oxopropanoic acid (PIN)

P-65.6 SALTS AND ESTERS

- P-65.6.1 General methodology
- P-65.6.2 Salts
- P-65.6.3 Esters, lactones, and related compounds

P-65.6.1 General methodology

Neutral salts and esters are both named using the name of the anion derived from the name of the acid. Anion names are formed by changing an '-ic acid' ending of an acid name to '-ate' and an '-ous acid' ending of an acid name to '-ite'. Then, salts are named using the names of cations, and esters the names of organyl groups, cited as separate words in front of the name of the anion.

P-65.6.2 Salts

P-65.6.2.1 Neutral salts of acids are named by citing the name of the cation(s) followed by the name of the anion (see P-72.2.2.2) as a separate word. Different cations are cited in alphabetical order. Formation of salts is a functionalization and not a substitution. Thus, all retained names, both those used as preferred IUPAC names and those used only for general nomenclature, can be used without restriction. This rule applies equally to acids expressed by suffixes and carbonic, cyanic, oxalic, and polycarbonic acids.

Examples:

$\mathrm{CH_3\text{-}CH_2\text{-}CH_2\text{-}COO^{-}\ K^{+}}$
potassium butanoate (PIN)

$\mathrm{CH_3\text{-}CH_2\text{-}CS\text{-}S^{-}\ Na^{+}}$
sodium propane(dithioate) (PIN)

$\mathrm{(CH_3\text{-}COO^{-})_2\ Ca^{2+}}$
calcium diacetate (PIN)

$\mathrm{C_6H_5\text{-}SO\text{-}O^{-}\ Na^{+}}$
sodium benzenesulfinate (PIN)

$\mathrm{K^{+}\ {}^{-}OOC\text{-}CH_2\text{-}CH_2\text{-}COO^{-}\ Na^{+}}$
potassium sodium butanedioate (PIN)
potassium sodium succinate

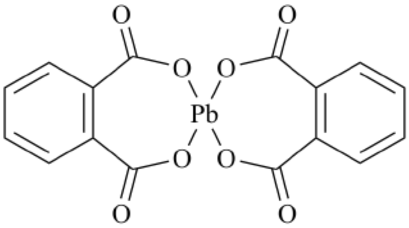
$\mathrm{NH_4^{+}\ {}^{-}OOC\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}COO^{-}\ K^{+}}$
ammonium potassium hexanedioate (PIN)
ammonium potassium adipate

$\mathrm{C(O)O_2^{2-}\ 2Na^{+}}$
disodium carbonate (PIN)

$\mathrm{(CH_3\text{-}COO^{-})_4\ Ge^{4+}}$
germanium tetraacetate (PIN)

P-65.6.2.2 Cyclic salts are named as heterocycles

Example:



3,3′-spirobi[[2,4,3]benzodioxaplumbepine]-1,1′,5,5′-tetrone (PIN)

P-65.6.2.3 Acid salts

P-65.6.2.3.1 Acid salts of polybasic organic acids are named in two ways:

(1) by substitutive nomenclature in which the free acid is cited as a prefix to the name of the anion;

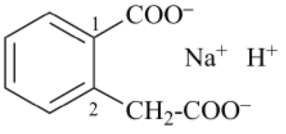
(2) in the same way as the neutral salts, the remaining acid hydrogen atom(s) being indicated by the word ‘hydrogen’ (preceded by a numerical prefix, ‘di’, ‘tri’, etc., as appropriate) inserted as a separate word between the name(s) of the cation(s) and the name of the anion. When required, cations are cited in names in alphabetical order.

Method (1) generates preferred IUPAC names, except when the structure of the acid salt is unknown. Anionic substituents, such as $\mathrm{–COO^{-}}$, $\mathrm{–SO_3^{-}}$, $\mathrm{–SO_2^{-}}$ are described by the prefix names ‘carboxylato’, ‘sulfonato’, and ‘sulfinato’, respectively, and similarly for the corresponding selenium and tellurium acids.

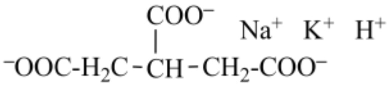
Examples:

$\mathrm{HOOC\text{-}[CH_2]_5\text{-}COO^{-}\ K^{+}}$
(1) potassium 6-carboxyhexanoate (PIN)
(2) potassium hydrogen heptanedioate

$\mathrm{HOOC\text{-}CH_2\text{-}CH_2\text{-}COO^{-}\ NH_4^{+}}$
(1) ammonium 3-carboxypropanoate (PIN)
(2) ammonium hydrogen butanedioate
ammonium hydrogen succinate



(2) sodium hydrogen 2-(carboxylatomethyl)benzoate (PIN)



$$^{-}OOC\text{-}H_2C\text{-}\overset{\overset{\displaystyle COO^-}{|}}{C}H\text{-}CH_2\text{-}COO^- \quad Na^+ \quad K^+ \quad H^+$$

(2) potassium sodium hydrogen propane-1,2,3-tricarboxylate (PIN)

$(HOOC\text{-}CH_2\text{-}CH_2\text{-}COO^-)_3\ Sb^{3+}$
(1) antimony tris(3-carboxypropanoate) (PIN)
(2) antimony tris(hydrogen butanedioate)

P-65.6.2.3.2 Preferred IUPAC names of acid salts of organic derivatives of polybasic inorganic oxoacids (including carbonic) are named by method (2).

Examples:

$HO\text{-}CO\text{-}O^-\ Na^+$
sodium hydrogen carbonate (PIN)

$CH_3\text{-}P(O)(O^-)_2\ K^+\ H^+$
potassium hydrogen methylphosphonate (PIN)

Note: In the nomenclature of inorganic chemistry (IR-8.4, ref. 12), the term ‘hydrogen’ is written directly in front of the name of the anion, without a space, to indicate that it is part of the anion.

Example:

$P(O)(O^-)^{3-}\ Na^+\ 2\ H^+$
sodium dihydrogenphosphate

P-65.6.3 Esters, lactones, and related compounds

P-65.6.3.1 Definitions
P-65.6.3.2 General methodology
P-65.6.3.3 Peferred IUPAC names for esters
P-65.6.3.4 Pseudoesters
P-65.6.3.5 Cyclic esters
P-65.6.3.6 Acylals

P-65.6.3.1 Definitions

P-65.6.3.1.1 Esters of organic oxoacids, R-C(O)-O-R′ (R can be H) or $R\text{-}S(O)_x\text{-}O\text{-}R$ ($R \neq H$) or chalcogen analogues, are compounds formally derived from an organic oxoacid R-C(O)-OH (R can be H) or $R\text{-}S(O)_x\text{-}OH$ ($R \neq H$) and an alcohol, phenol, heterol, or enol by a formal loss of water from an acidic hydroxy group of the former and a hydroxy group of the latter. By extension, they are ‘acyl’ derivatives of alcohols, etc. Esters derived from chalcogen analogs of organic oxoacids and chalcogen analogues of alcohols (thiols, selenols, tellurols), phenols, heterols, and enols, i.e., acyl derivatives of chalcogen analogues of alcohols (thiols, selenols, tellurols), phenols, heterols, and enols, are also included.

For esters derived from inorganic oxoacids, see Section P-67.

P-65.6.3.1.2 Pseudoesters are compounds having the generic formula $R\text{-}E(=O)_x(OZ)$ and chalcogen analogues where $x = 1$ or 2 and Z is not a carbon atom but an element from the following list: B, Al, In, Ga, Tl, Si, Ge, Sn, Pb, N(cyclic), P, As, Sb, Bi. Pseudoesters are ranked as esters in the seniority order of classes (see P-41).

Examples:

$CH_3\text{-}CO\text{-}O\text{-}Si(CH_3)_3$
trimethylsilyl acetate (PIN)

$CH_3\text{-}CH_2\text{-}SO_2\text{-}S\text{-}Ge(CH_3)_3$
S-(trimethylgermyl) ethanesulfonothioate (PIN)

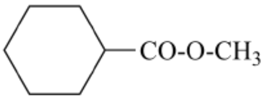
P-65.6.3.2 General methodology

P-65.6.3.2.1 All preferred IUPAC names for esters are named by functional class nomenclature.

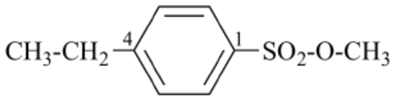
Examples:

$CH_3\text{-}CO\text{-}O\text{-}CH_2\text{-}CH_3$
ethyl acetate (PIN)

$CH_3\text{-}O\text{-}CO\text{-}CH_2\text{-}CH_2\text{-}CO\text{-}O\text{-}CH_2\text{-}CH_3$
ethyl methyl butanedioate (PIN)



methyl cyclohexanecarboxylate (PIN)



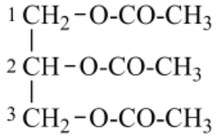
methyl 4-ethylbenzene-1-sulfonate (PIN)

P-65.6.3.2.2 Multiplicative functional class names for esters

In functional class nomenclature for esters the multiplicative operation (P-13.6.2) is used to name assemblies of identical parent anionic components linked by a di- or multivalent 'hydroxylic' component.

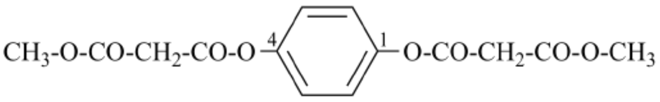
> A change occurs in the multiplicative operation applied to esters from previous recommendations. The bi- or polyvalent functional class name is cited as the organyl (alkanediyl, arylene, etc.) group cited immediately before the name of the acid component denoted by the anion name derived from the appropriate acid (see P-72.2.2.2.1) rather than alphabetically along with other monovalent organyl groups as was done in earlier recommendations.

Examples:

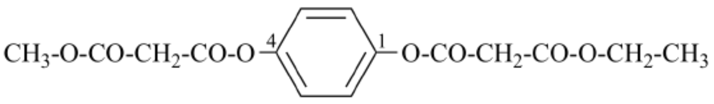


$$\begin{array}{ll} ^{1} & CH_2\text{-}O\text{-}CO\text{-}CH_3 \\ & | \\ ^{2} & CH\text{-}O\text{-}CO\text{-}CH_3 \\ & | \\ ^{3} & CH_2\text{-}O\text{-}CO\text{-}CH_3 \end{array}$$

propane-1,2,3-triyl triacetate (PIN)



dimethyl 1,4-phenylene dipropanedioate (PIN)
1,4-phenylene di(methyl propanedioate)



ethyl methyl 1,4-phenylene dipropanedioate (PIN)

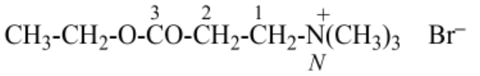
P-65.6.3.2.3 Esters cited as prefixes

When, in an ester with the general structure R-CO-O-R′ or R-S(O)$_x$-O-R′, another group is present that has priority for citation as the principal group or when all ester groups cannot be described by the methods prescribed for naming esters, an ester group is indicated by prefixes as 'acyloxy' for the group R-CO-O–, and 'alkoxy...oxo', '(alkyloxy)...oxo', '(alkanyloxy)...oxo', 'alkoxycarbonyl', '(alkyloxy)carbonyl' or '(alkanyloxy)carbonyl' for the group –CO-OR′.

The systematic name 'acetyloxy' is preferred to the contracted name 'acetoxy' that may be used in general nomenclature.

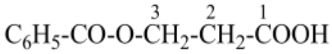
Seniority for numbering follows that for acids, for which see P-65.1.2.3.

Examples:



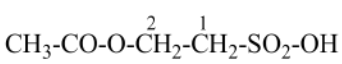
$$CH_3\text{-}CH_2\text{-}O\text{-}\overset{3}{C}O\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}H_2\text{-}\underset{N}{\overset{+}{N}}(CH_3)_3 \quad Br^-$$

3-ethoxy-*N*,*N*,*N*-trimethyl-3-oxopropan-1-aminium bromide (PIN)
[2-(ethoxycarbonyl)ethyl]tri(methyl)ammonium bromide
(3-ethoxy-3-oxopropyl)tri(methyl)azanium bromide



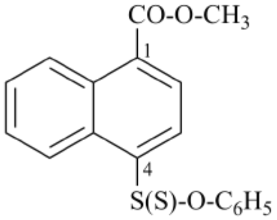
$$C_6H_5\text{-}CO\text{-}O\text{-}\overset{3}{C}H_2\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}OOH$$

3-(benzoyloxy)propanoic acid (PIN)
3-[(phenylcarbonyl)oxy]propanoic acid

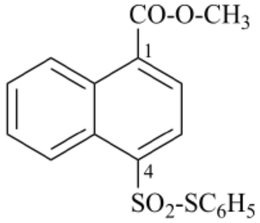


$$CH_3\text{-}CO\text{-}O\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}H_2\text{-}SO_2\text{-}OH$$

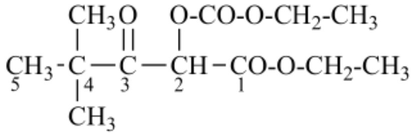
2-(acetyloxy)ethane-1-sulfonic acid (PIN)
2-acetoxyethanesulfonic acid



methyl 4-(phenoxysulfinothioyl)naphthalene-1-carboxylate (PIN)

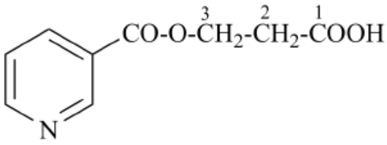


methyl 4-[(phenylsulfanyl)sulfonyl]naphthalene-1-carboxylate (PIN)

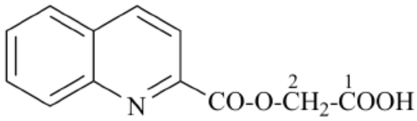


$$\begin{array}{ccccccc}
 & CH_3 & & O & & O\text{-}CO\text{-}O\text{-}CH_2\text{-}CH_3 & \\
 & | & & \| & & | & \\
CH_3\text{-} & C & - & C & - & CH & \text{-}CO\text{-}O\text{-}CH_2\text{-}CH_3 \\
5 & |\,4 & & 3 & & 2 & 1 \\
 & CH_3 & & & & &
\end{array}$$

ethyl 2-[(ethoxycarbonyl)oxy]-4,4-dimethyl-3-oxopentanoate (PIN)



3-[(pyridine-3-carbonyl)oxy]propanoic acid (PIN)
3-(nicotinoyloxy)propanoic acid



[(quinoline-2-carbonyl)oxy]acetic acid (PIN)
[(quinolin-2-ylcarbonyl)oxy]acetic acid;
(see P-65.4.1 for naming acyl groups derived from acids)

P-65.6.3.3 Preferred IUPAC names for esters

P-65.6.3.3.1 Monoesters
P-65.6.3.3.2 Polyesters derived from a single acid component
P-65.6.3.3.3 Polyesters formed from a single ‘alcoholic’ component
P-65.6.3.3.4 Polyesters derived from multiple acid components and multiple ‘alcoholic’ components
P-65.6.3.3.5 Partial esters from polybasic acids and their salts
P-65.6.3.3.6 Substitutive nomenclature is senior to functional class nomenclature for preferred IUPAC names for esters
P-65.6.3.3.7 Esters of acids modified by functional replacement nomenclature

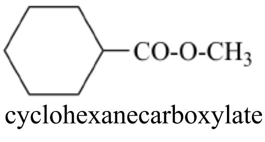
P-65.6.3.3.1 Monoesters

Monoesters formed from a monobasic acid and a ‘monohydroxylic’ component are named systematically by placing the ‘hydroxylic’ component denoted by an organyl group (alkyl, aryl, etc.) in front of the name of the acid component expressed as an anion derived from the appropriate acid (see P-72.2.2.2.1).

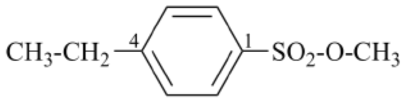
Examples:

$CH_3CO\text{-}O\text{-}CH_2\text{-}CH_3$
ethyl acetate (PIN)

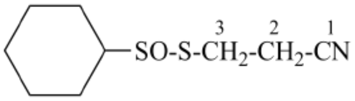
$CH_3\text{-}[CH_2]_6\text{-}CO\text{-}O\text{-}C(CH_3)_3$
tert-butyl octanoate (PIN)
1,1-dimethylethyl octanoate



methyl cyclohexanecarboxylate (PIN)



methyl 4-ethylbenzene-1-sulfonate (PIN)



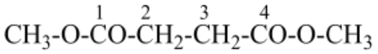
S-(2-cyanoethyl) cyclohexanesulfinothioate (PIN)
{not 3-[(cyclohexanesulfinyl)sulfanyl]propanenitrile
nor 3-[(cyclohexylsulfinyl)sulfanyl]propanenitrile;
see P-65.4.1 for naming acyl groups derived from acids}

P-65.6.3.3.2 Polyesters derived from a single acid component

P-65.6.3.3.2.1 Fully esterified acids derived from a single acid are systematically named by placing the name(s) of the hydroxylic component denoted by an organyl group(s) (alkyl, aryl, etc.) as separate word(s) in front of the name of the acid component denoted by the anion name derived from the appropriate acid (see P-72.2.2.2.1). Multiplicative prefixes are used to denote a multiplicity of identical organyl groups; different organyl groups are cited in alphanumerical order (see P-14.5). When necessary, locants are cited at the front of the organyl groups.

This rule applies equally to carboxylic, sulfonic, sulfinic, etc. acids.

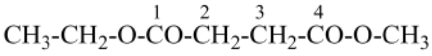
Examples:



$\mathrm{CH_3\text{-}O\text{-}\overset{1}{C}O\text{-}\overset{2}{C}H_2\text{-}\overset{3}{C}H_2\text{-}\overset{4}{C}O\text{-}O\text{-}CH_3}$

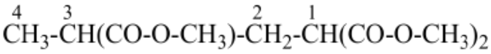
dimethyl butanedioate (PIN)
dimethyl succinate

$\mathrm{CH_3\text{-}CH_2\text{-}O\text{-}CO\text{-}CH_2\text{-}CO\text{-}O\text{-}CH_3}$
ethyl methyl propanedioate (PIN)
ethyl methyl malonate



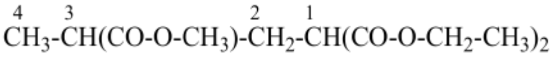
$\mathrm{CH_3\text{-}CH_2\text{-}O\text{-}\overset{1}{C}O\text{-}\overset{2}{C}H_2\text{-}\overset{3}{C}H_2\text{-}\overset{4}{C}O\text{-}O\text{-}CH_3}$

ethyl methyl butanedioate (PIN)



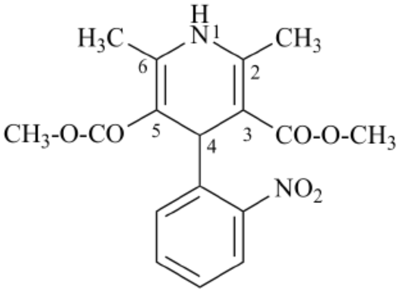
$\mathrm{\overset{4}{C}H_3\text{-}\overset{3}{C}H(CO\text{-}O\text{-}CH_3)\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}H(CO\text{-}O\text{-}CH_3)_2}$

trimethyl butane-1,1,3-tricarboxylate (PIN)

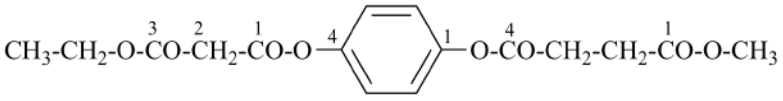


$\mathrm{\overset{4}{C}H_3\text{-}\overset{3}{C}H(CO\text{-}O\text{-}CH_3)\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}H(CO\text{-}O\text{-}CH_2\text{-}CH_3)_2}$

1,1-diethyl 3-methyl butane-1,1,3-tricarboxylate (PIN)



dimethyl 2,6-dimethyl-4-(2-nitrophenyl)-1,4-dihydropyridine-3,5-dicarboxylate (PIN)



4-[(3-ethoxy-3-oxopropanoyl)oxy]phenyl methyl butanedioate (PIN)
(not ethyl 4-[(4-methoxy-4-oxobutanoyl)oxy]phenyl propanedioate;
butanedioate is preferred to propandioate)

P-65.6.3.3.2.2 Polyester names formed by multiplicative nomenclature

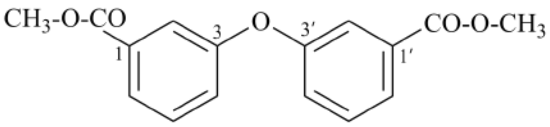
P-65.6.3.3.2.2.1 Esters of acid components whose preferred IUPAC names are derived using multiplicative nomenclature are named by two methods:

(1) all organyl components representing the ‘hydroxylic’ components are cited in front of the name of the multiplied acid component;

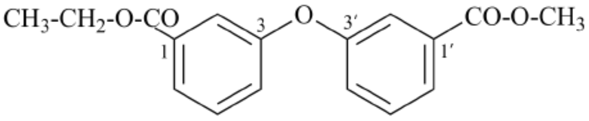
(2) for esters where both organyl components representing the ‘hydroxylic’ components are exactly the same are cited with the acid component preceded by a numerical term ‘bis-’, ‘tris-’, etc.

Method (1) leads to preferred IUPAC names.

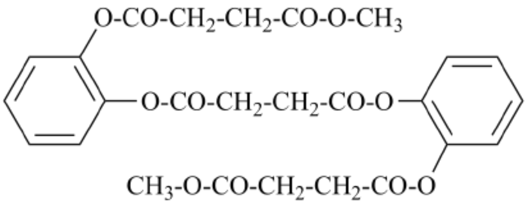
Examples:



(1) dimethyl 3,3′-oxydibenzoate (PIN)
(2) 3,3′-oxybis(methyl benzoate)



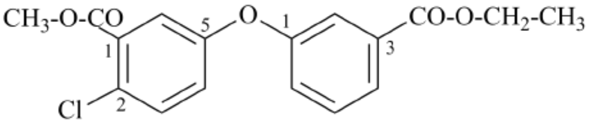
(1) ethyl methyl 3,3′-oxydibenzoate (PIN)



(1) dimethyl butanedioylbis(oxy-2,1-phenylene)dibutanedioate (PIN)
(not bis{2-[(4-methoxy-4-oxobutanoyl)oxy]phenyl} butanedioate;
the PIN expresses two parent dicarboxylic acids)
(2) butanedioylbis(oxy-2,1-phenylene) bis(methyl butanedioate)

P-65.6.3.3.2.2.2 Esters that do not qualify for multiplicative names as described above are named as monoesters and other ester components are expressed as prefixes by substitutive nomenclature. A multiplicative name could be used in general nomenclature [see P-15.3.2 and P-51.3.3].

Example:



methyl 2-chloro-5-[3-(ethoxycarbonyl)phenoxy]benzoate (PIN)
(not ethyl 3-[4-chloro-3-(methoxycarbonyl)phenoxy]benzoate;
the parent structure of the PIN has more substituents)
1′-ethyl 1-methyl 6-chloro-3,3′-oxydibenzoate
(this multiplicative name is acceptable only in general nomenclature.

P-65.6.3.3.3 Polyesters formed from a single ‘alcoholic’ component

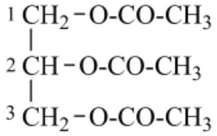
Esters derived from a single ‘polyhydroxylic’ component are named by placing the name of the ‘polyhydroxylic’ component denoted by a multivalent organyl group (alkyl, aryl, etc.) in front of the name(s) of the acid component denoted by the anion names derived from the appropriate acid(s) (see P-72.2.2.2.1).

P-65.6.3.3.3.1 When anions are identical functional class multiplicative nomenclature is used. Names are formed by citing the multivalent group, the multiplicative prefix, and the multiplied anionic component name. Multiplicative prefixes ‘di’, ‘tri’, etc. are used when anions are unsubstituted; when substituted, prefixes ‘bis’, ‘tris’, etc. are used.

Examples:

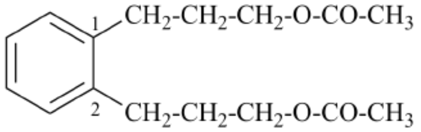
$CH_3\text{-}CO\text{-}O\text{-}\overset{1}{C}H_2\text{-}\overset{2}{C}H_2\text{-}O\text{-}CO\text{-}CH_3$
ethane-1,2-diyl diacetate (PIN)

$ClCH_2\text{-}CO\text{-}O\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}O\text{-}CO\text{-}CH_2Cl$
propane-1,3-diyl bis(chloroacetate) (PIN)



$$\begin{array}{l} {}^1\,CH_2\text{-}O\text{-}CO\text{-}CH_3 \\ \quad | \\ {}^2\,CH\text{-}O\text{-}CO\text{-}CH_3 \\ \quad | \\ {}^3\,CH_2\text{-}O\text{-}CO\text{-}CH_3 \end{array}$$

propane-1,2,3-triyl triacetate (PIN)



1,2-phenylenedi(propan-3,1-yl) diacetate [PIN; see P-15.3.0 (2) and P-51.3.1]

P-65.6.3.3.3.2 When anions are different, two methods are used:

(1) names of anions are cited in alphanumerical order preceded by a locant, when required; multiplicative prefixes are used to denote a multiplicity of identical anionic components;

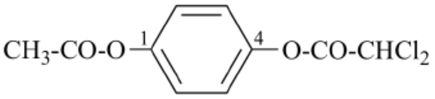
(2) one anion is chosen as principal anion and all other ester groups are expressed as prefixes in the name of the organyl group. The seniority order of anions is corresponding to that of acids (see seniority order of acids in P-41).

Method (1) generates preferred IUPAC names but names formed by using method (2) are acceptable in general nomenclature.

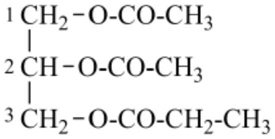
Examples:

$\mathrm{HCO\text{-}O\text{-}CH_2\text{-}O\text{-}CO\text{-}CH_3}$

(1) methylene acetate formate (PIN)
(2) (formyloxy)methyl acetate

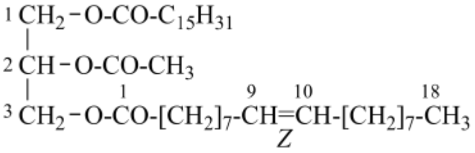


(1) 1,4-phenylene acetate dichloroacetate (PIN)
(2) 4-(acetyloxy)phenyl dichloroacetate



$$\begin{array}{l} {}^{1}\mathrm{CH_2-O\text{-}CO\text{-}CH_3} \\ \;| \\ {}^{2}\mathrm{CH-O\text{-}CO\text{-}CH_3} \\ \;| \\ {}^{3}\mathrm{CH_2-O\text{-}CO\text{-}CH_2\text{-}CH_3} \end{array}$$

(1) propane-1,2,3-triyl 1,2-diacetate 3-propanoate (PIN)
(2) 2,3-bis(acetyloxy)propyl propanoate



$$\begin{array}{l} {}^{1}\mathrm{CH_2-O\text{-}CO\text{-}C_{15}H_{31}} \\ \;| \\ {}^{2}\mathrm{CH-O\text{-}CO\text{-}CH_3} \\ \;| \\ {}^{3}\mathrm{CH_2-O\text{-}\overset{1}{C}O\text{-}[CH_2]_7\text{-}\overset{9}{C}H\underset{Z}{=}\overset{10}{C}H\text{-}[CH_2]_7\text{-}\overset{18}{C}H_3} \end{array}$$

(1) propane-1,2,3-triyl 2-acetate 1-hexadecanoate 3-[(9*Z*)-octadec-9-enoate] (PIN)
(2) 2-(acetyloxy)-3-(hexadecanoyloxy)propyl (9*Z*)-octadec-9-enoate

P-65.6.3.3.4 Polyesters derived from multiple acids and multiple ‘alcoholic’ components

Multiplicative nomenclature, skeletal replacement (‘a’) nomenclature, or phane nomenclature is used when specific conditions for their use exist and are fulfilled.

P-65.6.3.3.4.1 Polyester names formed by using functional class multiplicative nomenclature

Symmetrical esters are named by including the organyl constituent in the multiplied anion component name. When this condition is not fulfilled, in unsymmetrical esters, the organyl constituents are cited at the beginning of the name, in alphanumerical order.

Example:

$\mathrm{CH_3\text{-}O\text{-}CO\text{-}CH_2\text{-}CH_2\text{-}CO\text{-}O\text{-}CH_2\text{-}CH_2\text{-}O\text{-}CO\text{-}CH_2\text{-}CH_2\text{-}CO\text{-}O\text{-}CH_3}$

dimethyl ethane-1,2-diyl dibutanedioate (PIN)
ethane-1,2-diyl bis(methyl butanedioate)

P-65.6.3.3.4.2 Polyester names formed by using substitutive nomenclature, and/or multiplicative nomenclature, and functional class nomenclature

Polyesters that cannot be named by functional class multiplicative nomenclature as described above, are named by using substitutive nomenclature to generate the names of the organyl substituents and those of the anions. When required, seniority of rings, ring systems, and chains; number and location of substituents; and alphanumerical order is applied in forming the alcoholic component of a functional class ester name (see P-41 through P-45):

Examples:

$$\mathrm{CH_3\text{-}O\text{-}\overset{4}{C}O\text{-}\overset{3}{C}H_2\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}O\text{-}O\text{-}\overset{1}{C}H_2\text{-}\overset{2}{C}H_2\text{-}O\text{-}CO\text{-}CH_3}$$

2-(acetyloxy)ethyl methyl butanedioate (PIN)
2-acetoxyethyl methyl butanedioate

$$\mathrm{CH_3\text{-}O\text{-}\overset{4}{C}O\text{-}[\overset{3\text{-}2}{C}H_2]_2\text{-}\overset{1}{C}O\text{-}O\text{-}[CH_2]_2\text{-}O\text{-}\overset{1}{C}O\text{-}[\overset{2\text{-}3}{C}H_2]_2\text{-}\overset{4}{C}O\text{-}O\text{-}[\overset{1\text{-}2}{C}H_2]_2\text{-}O\text{-}CO\text{-}CH_3}$$

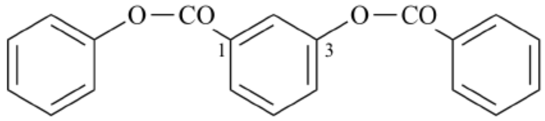
2-(acetyloxy)ethyl methyl ethane-1,2-diyl dibutanedioate (PIN)

$$\mathrm{CH_3\text{-}CO\text{-}O\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}H_2\text{-}O\text{-}CO\text{-}CH_2\text{-}CO\text{-}O\text{-}\overset{1}{C}H_2\text{-}\overset{2}{C}H_2\text{-}O\text{-}CO\text{-}CH_3}$$

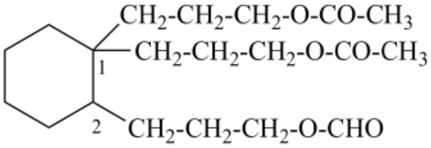
bis[2-(acetyloxy)ethyl] propanedioate (PIN)
propanedioylbis(oxyethane-2,1-diyl) diacetate

$$\mathrm{CH_3\text{-}CO\text{-}O\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}H_2\text{-}O\text{-}\overset{1}{C}O\text{-}\overset{2}{C}H_2\text{-}\overset{3}{C}H_2\text{-}\overset{4}{C}O\text{-}O\text{-}\overset{1}{C}H_2\text{-}\overset{2}{C}H_2\text{-}O\text{-}CO\text{-}CH_2\text{-}CH_3}$$

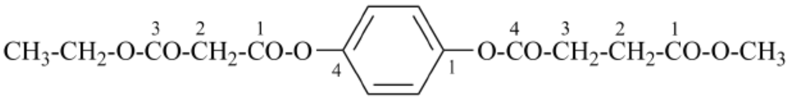
2-(acetyloxy)ethyl 2-(propanoyloxy)ethyl butanedioate (PIN)
butanedioylbis(oxyethane-2,1-diyl) acetate propanoate



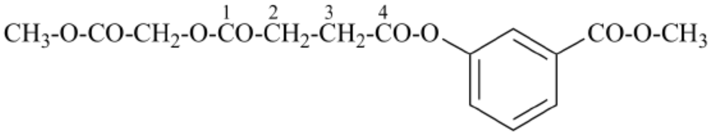
phenyl 3-(benzoyloxy)benzoate (PIN)
[not 3-(phenoxycarbonyl)phenyl benzoate;
the substituted benzoic acid is senior to the unsubstituted one; see P-45.2.1]


CH₂-CH₂-CH₂-O-CO-CH₃
CH₂-CH₂-CH₂-O-CO-CH₃
1
2
CH₂-CH₂-CH₂-O-CHO

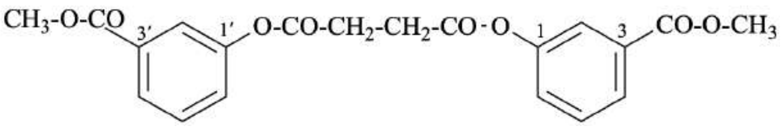
2-[3-(formyloxy)propyl]cyclohexane-1,1-diyldi(propane-3,1-diyl) diacetate (PIN)


3 2 1
CH₃-CH₂-O-CO-CH₂-CO-O
4
1
4 3 2 1
O-CO-CH₂-CH₂-CO-O-CH₃

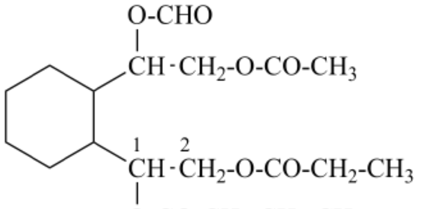
4-[(3-ethoxy-3-oxopropanoyl)oxy]phenyl methyl butanedioate (PIN)
(not ethyl 4-[(4-methoxy-4-oxobutanoyl)oxy]phenyl propanedioate;
butanedioic acid is preferred to propanedioic acid


1 2 3 4
CH₃-O-CO-CH₂-O-CO-CH₂-CH₂-CO-O
CO-O-CH₃

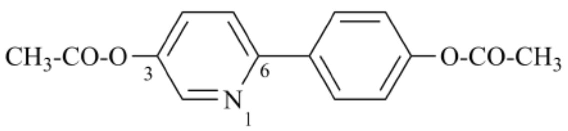
3-(methoxycarbonyl)phenyl 2-methoxy-2-oxoethyl butanedioate (PIN)
[not 2-methoxy-2-oxoethyl 3-(methoxycarbonyl)phenyl butanedioate;
3-(methoxycarbonyl)phenyl is alphabetically before 2-methoxy-2-oxoethyl; see P-14.5]


CH₃-O-CO
3′
1′
O-CO-CH₂-CH₂-CO-O
1
3
CO-O-CH₃

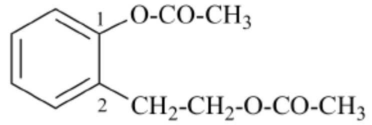
bis[3-(methoxycarbonyl)phenyl] butanedioate (PIN)
(not dimethyl 3,3′-[butanedioylbis(oxy)]dibenzoate;
a dicarboxylic acid is senior to two monocarboxylic acids)


O-CHO
CH-CH₂-O-CO-CH₃
1 2
CH-CH₂-O-CO-CH₂-CH₃
O-CO-CH₂-CH₂-CH₃

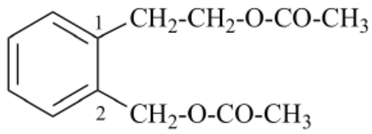
1-{2-[2-(acetyloxy)-1-(formyloxy)ethyl]cyclohexyl}ethane-1,2-diyl 1-butanoate 2-propanoate (PIN)



6-[4-(acetyloxy)phenyl]pyridin-3-yl acetate (PIN)
(not 4-[5-(acetyloxy)pyridin-2-yl]phenyl acetate;
the nitrogenous ring is senior to the carbocyclic ring)



2-[2-(acetyloxy)ethyl]phenyl acetate (PIN)
(not 2-[2-(acetyloxy)phenyl]ethyl acetate;
the ring is senior to the chain)



2-{2-[(acetyloxy)methyl]phenyl}ethyl acetate (PIN)
(not 2-{2-[(acetyloxy)ethyl]phenyl}methyl acetate;
the ethyl chain is senior to the methyl chain)

P-65.6.3.3.4.3 Polyester names formed by using functional class nomenclature and skeletal replacement (‘a’) nomenclature:

Examples:

$$CH_3\text{-}O\text{-}\overset{1}{C}O\text{-}CH_2\text{-}\overset{3}{C}O\text{-}\overset{4}{O}\text{-}CH_2\text{-}CH_2\text{-}\overset{7}{O}\text{-}\overset{8}{C}O\text{-}CH_2\text{-}\overset{10}{C}O\text{-}\overset{11}{O}\text{-}CH_2\text{-}CH_2\text{-}\overset{14}{O}\text{-}\overset{15}{C}O\text{-}CH_2\text{-}\overset{17}{C}O\text{-}O\text{-}CH_3$$

dimethyl 3,8,10,15-tetraoxo-4,7,11,14-tetraoxaheptadecane-1,17-dioate (PIN)
[a functional class name in which the anion segment is named by skeletal replacement (‘a’) nomenclature.]
dimethyl methylenebis(carbonyloxyethane-2,1-diyl) dipropanedioate (a functional class multiplicative name)

$$CH_3\text{-}O\text{-}\overset{1}{C}O\text{-}\overset{2}{[CH_2]_2}\text{-}\overset{4}{C}O\text{-}\overset{5}{O}\text{-}\overset{6\text{-}7}{[CH_2]_2}\text{-}\overset{8}{O}\text{-}\overset{9}{C}O\text{-}\overset{10\text{-}11}{[CH_2]_2}\text{-}\overset{12}{C}O\text{-}\overset{13}{O}\text{-}\overset{14\text{-}15}{[CH_2]_2}\text{-}\overset{16}{O}\text{-}\overset{17}{C}O\text{-}\overset{18\text{-}19}{[CH_2]_2}\text{-}\overset{20}{C}O\text{-}O\text{-}CH_3$$

dimethyl 4,9,12,17-tetraoxo-5,8,13,16-tetraoxaicosane-1,20-dioate (PIN)
[a functional class name in which the anion segment is named by skeletal replacement (‘a’) name]
dimethyl ethane-1,2-diylbis(carbonyloxyethane-2,1-diyl) dibutanedioate (a functional class multiplicative name)

$$CH_3\text{-}O\text{-}\overset{1}{C}O\text{-}\overset{2}{C}H_2\text{-}\overset{3}{C}O\text{-}\overset{4}{O}\text{-}\overset{5}{C}H_2\text{-}\overset{6}{O}\text{-}\overset{7\text{-}8}{[CH_2]_2}\text{-}\overset{9}{O}\text{-}\overset{10}{C}O\text{-}\overset{11}{C}H_2\text{-}\overset{12}{C}O\text{-}\overset{13}{O}\text{-}\overset{14\text{-}15}{[CH_2]_2}\text{-}\overset{16}{O}\text{-}\overset{17}{C}H_2\text{-}\overset{18}{O}\text{-}\overset{19}{C}O\text{-}\overset{20}{C}H_2\text{-}\overset{21}{C}O\text{-}O\text{-}CH_3$$

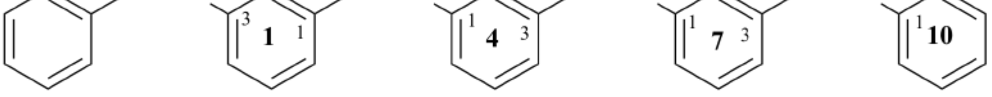
dimethyl 3,10,12,19-tetraoxo-4,6,9,13,16,18-hexaoxahenicosane-1,21-dioate (PIN)
dimethyl 6,8-dioxo-2,5,9,12-tetraoxatridecane-1,13-diyl dipropanedioate
[a functional class name in which the multiplying segment is named by skeletal replacement (‘a’) nomenclature]
dimethyl propanedioylbis(oxyethane-2,1-diyloxymethylene) dipropanedioate (a functional class multiplicative name)

$$CH_3\text{-}O\text{-}\overset{23}{C}O\text{-}\overset{22}{C}H_2\text{-}\overset{21}{C}O\text{-}\overset{20}{O}\text{-}\overset{19\text{-}18}{[CH_2]_2}\text{-}\overset{17}{O}\text{-}\overset{16}{C}O\text{-}\overset{15\text{-}14}{[CH_2]_2}\text{-}\overset{13}{C}O\text{-}\overset{12}{O}\text{-}\overset{11}{C}H_2\text{-}\overset{10}{O}\text{-}\overset{9}{C}O\text{-}\overset{8}{C}H_2\text{-}\overset{7}{C}O\text{-}\overset{6}{O}\text{-}\overset{5}{C}H_2\text{-}\overset{4}{O}\text{-}\overset{3}{C}O\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}O\text{-}O\text{-}CH_3$$

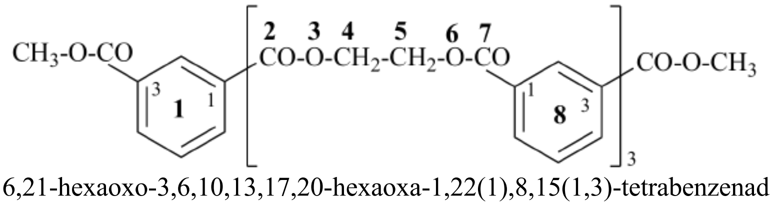
dimethyl 3,7,9,13,16,21-hexaoxo-4,6,10,12,17,20-hexaoxatricosane-1,23-dioate (PIN)
2-{[(methoxycarbonyl)acetyl]oxy}ethyl 3,5,9,11-tetraoxo-2,6,8,12-tetraoxatridecan-1-yl butanedioate
[a functional class name in which one alcoholic segment is named by skeletal replacement (‘a’) nomenclature]

P-65.6.3.3.4.4 Polyester names formed by using functional class nomenclature and phane nomenclature:

Examples:



phenyl 3,6,9-trioxo-2,5,8-trioxa-1,10(1),4,7(1,3)-tetrabenzenadecaphane-1^3-carboxylate (PIN)



dimethyl 2,7,9,14,16,21-hexaoxo-3,6,10,13,17,20-hexaoxa-1,22(1),8,15(1,3)-tetrabenzenadocosaphane-1^3,22^3-dicarboxylate (PIN)

P-65.6.3.3.5 Partial esters of polybasic acids and their salts are named by two methods:

(1) substitutively on the basis of the anion, the free acid group(s) and the ester group(s) being cited as prefixes;

(2) by the procedure for neutral esters and acid salts; the components present are cited in the order, cation, hydrocarbyl group, hydrogen, anion. Numerical locants and italic element symbols (see P-65.1.5.1) are added as necessary to provide specificity. The numbering of the polybasic acid is retained when the hydrogen method is applied to retained names.

Method (1) generates preferred IUPAC names.

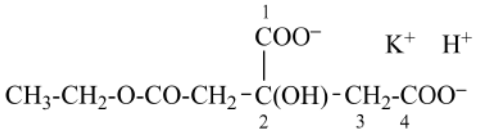
Examples:

$CH_3\text{-}CH_2\text{-}O\text{-}CO\text{-}CH_2\text{-}CH_2\text{-}COO^-\ Na^+$

(1) sodium 4-ethoxy-4-oxobutanoate (PIN)
(2) sodium ethyl succinate

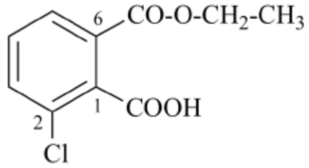
$CH_3\text{-}CH_2\text{-}S\text{-}\overset{4}{C}O\text{-}\overset{3}{C}H_2\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}\{O/S\}^-\ \ Li^+$

(1) lithium 4-(ethylsulfanyl)-4-oxobutanethioate (PIN)
(2) lithium *S*-ethyl butanebis(thioate)

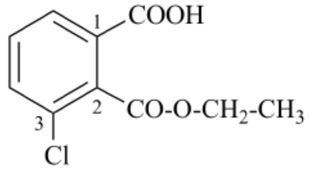


$$CH_3\text{-}CH_2\text{-}O\text{-}CO\text{-}CH_2-\underset{2}{\overset{\overset{1}{COO^-}\atop |}{C}}(OH)-\underset{3}{C}H_2\text{-}\underset{4}{C}OO^-\qquad K^+\ \ H^+$$

(1) potassium hydrogen 2-(2-ethoxy-2-oxoethyl)-2-hydroxybutanedioate (PIN)
(2) potassium 3-ethyl hydrogen 2-hydroxypropane-1,2,3-tricarboxylate
(2) potassium 3-ethyl hydrogen citrate
(the anionic ^-OOC– group is preferred to the ester group $CH_3\text{-}CH_2\text{-}O\text{-}CO$–)



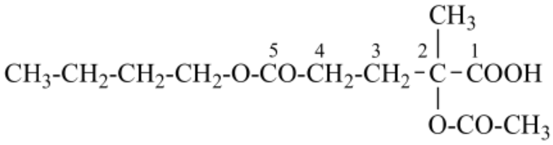
(1) 2-chloro-6-(ethoxycarbonyl)benzoic acid (PIN)
(2) 1-ethyl hydrogen 3-chlorobenzene-1,2-dicarboxylate
(2) 1-ethyl hydrogen 3-chlorophthalate



(1) 3-chloro-2-(ethoxycarbonyl)benzoic acid (PIN)
(2) 2-ethyl hydrogen 3-chlorobenzene-1,2-dicarboxylate
(2) 2-ethyl hydrogen 3-chlorophthalate

$CH_3\text{-}[CH_2]_3\text{-}O\text{-}\overset{5}{C}O\text{-}\overset{4}{C}H_2\text{-}\overset{3}{C}H_2\text{-}\overset{2}{C}H(CH_3)\text{-}\overset{1}{C}OOH$

(1) 5-butoxy-2-methyl-5-oxopentanoic acid (PIN)
(2) 5-butyl hydrogen 2-methylpentanedioate

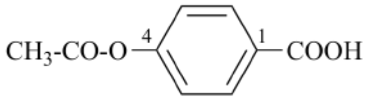


$$CH_3\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}O\text{-}\overset{5}{C}O\text{-}\overset{4}{C}H_2\text{-}\overset{3}{C}H_2-\underset{|\atop O\text{-}CO\text{-}CH_3}{\overset{CH_3\atop 2\,|}{C}}-\overset{1}{C}OOH$$

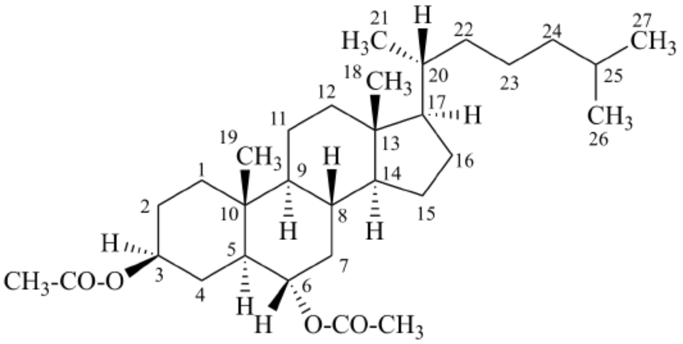
(1) 2-(acetyloxy)-5-butoxy-2-methyl-5-oxopentanoic acid (PIN)
(2) 5-butyl hydrogen 2-(acetyloxy)-2-methylpentanedioate

P-65.6.3.3.6 Substitutive nomenclature is senior to functional class nomenclature for preferred IUPAC for esters

Examples:



4-(acetyloxy)benzoic acid (PIN)
4-hydroxybenzoic acid acetate



5α-cholestane-3β,6α-diyl diacetate
5α-cholestane-3β,6α-diol diacetate

P-65.6.3.3.7 Esters of acids modified by functional replacement nomenclature

P-65.6.3.3.7.1 With the exception of retained names, polycarbonic acids and cyanic acid that are described in P-65.6.3.3.7.2, names of esters are all derived from acids modified by functional replacement whose substitutive names are systematically formed, as indicated in sections P-65.1.3 through P-65.1.7.

Structural specification for esters of thio-, seleno- or tellurocarboxylic acids, thio-, seleno-, or tellurosulfonic acids and sulfinic acids and their peroxy analogues is provided by the appropriate italic element symbol, such as *S*, *O*, or *SO*, prefixed to the name of the organyl group.

Examples:

CH_3-$[CH_2]_4$-CO-S-CH_2-CH_3
S-ethyl hexanethioate (PIN)

CH_3-$[CH_2]_4$-CSe-O-CH_2-CH_3
O-ethyl hexaneselenoate (PIN)

CH_3-C(=NH)-O-CH_3
methyl ethanimidate (PIN)
methyl acetimidate

CH_3-CH_2-C(=N-NH_2)-O-C_2H_5
ethyl propanehydrazonate (PIN)
ethyl propionohydrazonate

C_6H_5-C(=NH)-S-CH_3
methyl benzenecarboximidothioate (PIN)

C_6H_5-C(=N-SH)-S-CH_2-CH_3
ethyl *N*-sulfanylbenzenecarboximidothioate (PIN)

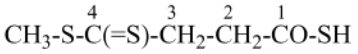
C_6H_5-CO-S-O-CH_3
SO-methyl benzene(carbothioperoxoate) (PIN)

CH_3-CH_2-SO_2-O-S-C_2H_5
OS-ethyl ethanesulfono(thioperoxoate) (PIN)

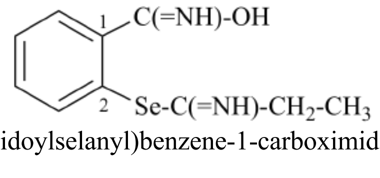
CH_3-S-CO-CO-S-CH_3
S,*S*-dimethyl ethanebis(thioate) (PIN)

In the presence of a characteristic group having seniority for citation as suffix, an ester group is indicated by preferred prefixes in accordance with the type of attachment of the substituent group, such as 'acylsulfanyl' for the group –S-CO-R, or '(alkylsulfanyl)carbonothioyl', or '(alkylsulfanyl)...sulfanylidene' for the group –CS-SR.

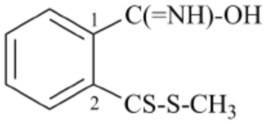
Examples:


$CH_3\text{-}S\text{-}\overset{4}{C}(=S)\text{-}\overset{3}{C}H_2\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}O\text{-}SH$

4-(methylsulfanyl)-4-sulfanylidenebutanethioic *S*-acid (PIN)



2-(propanimidoylselanyl)benzene-1-carboximidic acid (PIN)



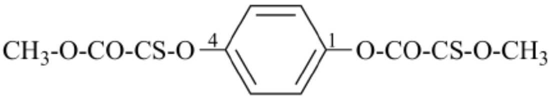
2-[(methylsulfanyl)carbonothioyl]benzene-1-carboxamidic acid (PIN)

$\mathrm{CH_3\text{-}O\text{-}\overset{1}{C}S\text{-}\overset{2}{C}(=NH)\text{-}S\text{-}CH_2\text{-}CH_3}$

O-methyl (ethylsulfanyl)(imino)ethanethioate (PIN)

$\mathrm{CH_3\text{-}S\text{-}\overset{1}{C}O\text{-}\overset{2}{C}S\text{-}S\text{-}CH_2\text{-}CH_3}$

S-methyl (ethylsulfanyl)(sulfanylidene)ethanethioate (PIN)



4-{[methoxy(oxo)ethanethioyl]oxy}phenyl methoxy(sulfanylidene)acetate (PIN)
[not *O*-methyl (4-{[methoxy(oxo)ethanethioyl]oxy}phenoxy)(oxo)ethanethioate;
a carboxylic acid is preferred to a thiocarboxylic acid;
not methyl (4-{[methoxy(sulfanylidene)acetyl]oxy}phenoxy)(sulfanylidene)acetate;
the PIN is lower in alphanumerical order)

P-65.6.3.3.7.2 Esters of carbonic acid, cyanic acid, and polycarbonic acids modified by functional replacement.

P-65.6.3.3.7.2.1 Names of acids modified by functional replacement are used to generate preferred IUPAC names of corresponding esters. Element symbols *O*, *S*, etc. and locants are used to designate the location of organyl groups.

Examples:

$\mathrm{CH_3\text{-}S\text{-}\overset{1}{C}O\text{-}\overset{2}{O}\text{-}\overset{3}{C}O\text{-}O\text{-}CH_2\text{-}CH_3}$

3-ethyl 1-*S*-methyl 1-thiodicarbonate (PIN)

CH_3-S-CS-O-CH_3

O,*S*-dimethyl carbonodithioate (PIN)

$(CH_3)_2$CH-S-CN

propan-2-yl thiocyanate (PIN)

P-65.6.3.3.7.2.2 In the presence of a characteristic group having seniority for citation as suffix, an ester group is indicated by appropriate prefixes in accordance with the type of attachment of the substituent group.

Examples:

CH_3-S-CS-CO-O-CH_2-CS-SH

{[(methylsulfanyl)(sulfanylidene)acetyl]oxy}ethane(dithoic acid) (PIN)

NC-S-CH_2-CH_2-CO-S-CH_2-CH_3

S-ethyl 3-(thiocyanato)propanethioate (PIN)

HS-CO-O-CS-O-CH_2-CH_2-COOH

3-({[(sulfanylcarbonyl)oxy]carbonothioyl}oxy)propanoic acid (PIN)

P-65.6.3.4 Pseudoesters

Compounds having the generic formula R-CO-O-E, where E is not a carbon atom nor an acyl group belong to this class (see P-65.6.3.1.2). Functional class names are constructed in the manner used for esters.

P-65.6.3.4.1 When 'E', in R-CO-O-E, is an element from the following list: B, Al, In, Ga, Tl, Si, Ge, Sn, Pb, N(cyclic), P, As, Sb, Bi, the pseudoester is named as a traditional ester, unless other names must be selected in accordance with the seniority order of classes, in decreasing order: salts > acids > anhydrides > esters. For anhydrides, see P-65.7.

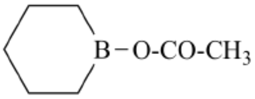
Examples:

CH_3-CO-O-Si$(CH_3)_3$

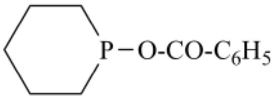
trimethylsilyl acetate (PIN)

CH_3-CH_2-SO_2-S-Ge$(CH_3)_3$

S-(trimethylgermyl) ethanesulfonothioate (PIN)



borinan-1-yl acetate (PIN)



phosphinan-1-yl benzoate (PIN)

$(CH_3\text{-}CO\text{-}O)_3B$
triacetic boric trianhydride (PIN)

$H_2P\text{-}O\text{-}CO\text{-}CH_3$
acetic phosphinous anhydride (PIN)

$(CH_3)_2N\text{-}O\text{-}CO\text{-}CH_3$
1-[(dimethylamino)oxy]ethan-1-one (PIN)
O-acetyl-*N*,*N*-dimethylhydroxylamine
(hydroxylamine is a preselected name; see P-68.3.1.1.1)

$CH_3\text{-}CO\text{-}O\text{-}P(CH_3)_2$
acetic dimethylphosphinous anhydride (PIN; see P-67.1.3.3)

P-65.6.3.4.2 When 'E' is an element belonging to Group 16, the pseudoester is named as a pseudoketone (see P-68.4.2.4)

Example:

$CH_3\text{-}CH_2\text{-}CH_2\text{-}CO\text{-}S\text{-}OO\text{-}CH_3$
[1-(methylperoxy)sulfanyl]butan-1-one (PIN)
(not *S*-methylperoxyl butanethioate)

P-65.6.3.5 Cyclic esters

Compounds that may be considered as derived from hydroxy carboxylic acids or hydroxy sulfonic acids by loss of water intramolecularly are classified as 'lactones' and 'sultones', respectively. For these compounds heterocyclic names are preferred IUPAC names. Names derived from corresponding hydroxy acids are not recommended, but may be used in general nomenclature.

P-65.6.3.5.1 Lactones

Intramolecular esters of hydroxy carboxylic acids are 'lactones' and are named in three ways.

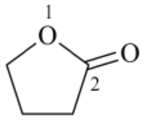
(1) as heterocyclic pseudoketones by adding the suffix 'one', 'dione', 'thione', etc. and the appropriate multiplicative prefixes to the name of the heterocyclic parent hydride;

(2) by changing the 'ic acid' ending of a systematic 'oic acid' name for the nonhydroxylated parent acid to 'lactone', and inserting a locant designating the position of the hydroxy group between the 'o' and 'lactone';

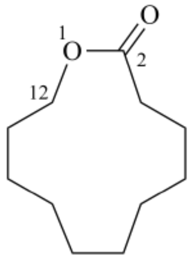
(3) by citing the term 'carbolactone' denoting the group –O-CO– in a ring or ring system after the name of the appropriate parent hydride preceded by a pair of locants describing the points of attachment of the carbonyl group and the oxygen atom, respectively; the locant of the carbonyl group is cited first, and, if there is a choice, is the lower locant. Multiplying prefixes and pairs of locants separated by a colon are used to indicate two or more carbolactone rings.

Method (1) gives preferred IUPAC names.

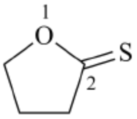
Examples:



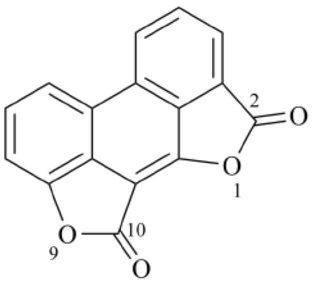
oxolan-2-one (PIN)
tetrahydrofuran-2-one
butano-4-lactone
(not γ-butyrolactone)



1-oxacyclododecan-2-one (PIN)
undecano-11-lactone



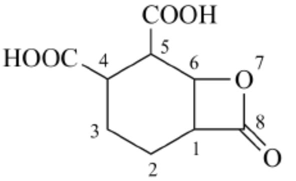
oxolane-2-thione (PIN)



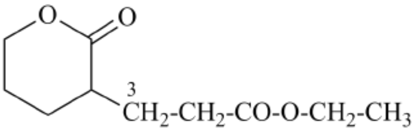
phenanthro[1,10-*bc*:9,8-*b*′*c*′]difuran-2,10-dione (PIN)
phenanthrene-1,10:9,8-dicarbolactone

A lactone, as a pseudoketone, ranks lower in the seniority of classes than an acid or an ester, but higher than an alcohol, amine, or imine.

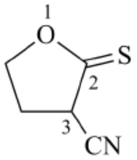
Examples:



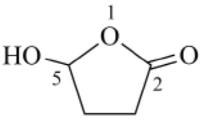
8-oxo-7-oxabicyclo[4.2.0]octane-4,5-dicarboxylic acid (PIN)
2-oxohexahydro-2*H*-benzooxete-5,6-dicarboxylic acid
(a preferred ring fusion name must have a fusion site and at least two rings of five or more members, see P-52.2.4.1)



ethyl 3-(2-oxooxan-3-yl)propanoate (PIN)
ethyl 3-(2-oxo-3,4,5,6-tetrahydro-2*H*-pyran-3-yl)propanoate
(the saturated Hantzsch-Widman name is preferred to the hydrogenated retained name, see P-54.4.2)



2-sulfanylideneoxolane-3-carbonitrile (PIN)



5-hydroxyoxolan-2-one (PIN)

P-65.6.3.5.2 Sultones and sultines are intramolecular esters of hydroxy sulfonic acids and sulfinic acids, respectively, and may be named in three ways:

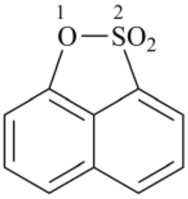
(1) as heterocyclic heterones by adding the suffix ‘one’, ‘dione’, ‘thione’, etc. and the appropriate multiplicative prefixes to the name of the heterocyclic parent hydride;

(2) by citing the term ‘sultone’ or ‘sultine’ denoting the –O-SO$_2$– or –O-SO– group in a ring or ring system after the name of the appropriate parent hydride preceded by a pair of locants describing the points of attachment of the sulfonyl or sulfinyl group and the oxygen atom, respectively; the locant of the sulfonyl or sulfinyl group is cited first, and, if there is a choice, is the lower locant. Multiplicative prefixes and pairs of locants separated by a colon are used to indicate two or more sultone or sultine rings.

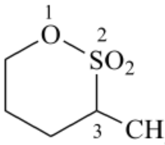
(3) as heterocycles according to functional class names using the class name ‘oxide’

Method (1) gives preferred IUPAC names.

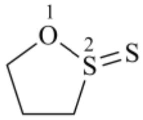
Examples:



2*H*-2λ^6-naphtho[1,8-*cd*][1,2]oxathiole-2,2-dione (PIN)
naphtho[1,8-*cd*][1,2]oxathiole 2,2-dioxide
naphthalene-1,8-sultone



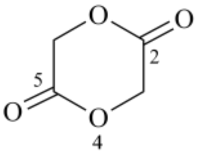
3-methyl-1,2λ^6-oxathiane-2,2-dione (PIN)
3-methyl-1,2-oxathiane 2,2-dioxide
pentane-2,5-sultone



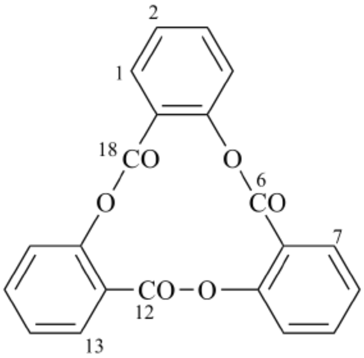
1,2λ^4-oxathiolane-2-thione (PIN)
1,2-oxathiolane 2-thiooxide

P-65.6.3.5.3 Lactides are cyclic esters derived by multiple esterification between two (or more) molecules of a hydroxy acid; they are named as heterocyclic compounds.

Examples:



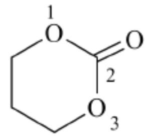
1,4-dioxane-2,5-dione (PIN)



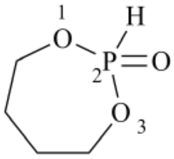
6*H*,12*H*,18*H*-tribenzo[*b*,*f*,*j*][1,5,9]trioxacyclododecine-6,12,18-trione (PIN)
(not trisalicylide)

P-65.6.3.5.4 Other cyclic esters derived from different hydroxy acids or from polybasic acids and polyhydroxy compounds are named as heterocycles.

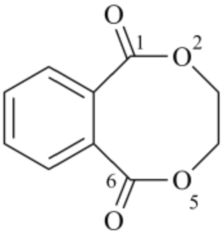
Examples:



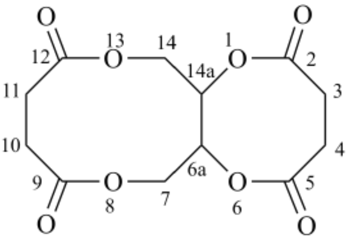
1,3-dioxan-2-one (PIN)



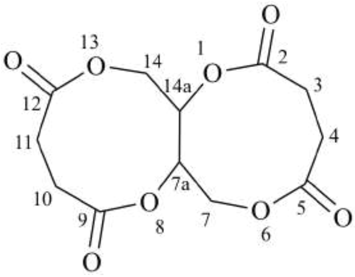
1,3,2λ^5-dioxaphosphepan-2-one (PIN)



3,4-dihydro-2,5-benzodioxocine-1,6-dione (PIN)
(not 3,4-dihydrobenzo[*f*][1,4]dioxocine-1,6-dione)



octahydro[1,4]dioxocino[2,3-*c*][1,6]dioxecine-2,5,9,12-tetrone (PIN)



octahydro[1,5]dioxonino[3,2-*b*][1,5]dioxonine-2,5,9,12-tetrone (PIN)

P-65.6.3.6 Acylals

Acylals are a class of compounds with the general structures R-CH(O-CO-R′)$_2$, RR′C(OCOR″)$_2$, etc. Specific compounds are named as esters.

Example:

$\overset{2}{C}H_3\text{-}\overset{1}{C}H(O\text{-}CO\text{-}CH_2\text{-}CH_2\text{-}CH_3)_2$

ethane-1,1-diyl dibutanoate (PIN)
(traditionally ethylidene dibutanoate)

P-65.7 ANHYDRIDES AND THEIR ANALOGUES

P-65.7.0 Introduction
P-65.7.1 Symmetric anhydrides
P-65.7.2 Mixed anhydrides
P-65.7.3 Thioanhydrides and other chalcogen analogues
P-65.7.4 Peroxyanhydrides and chalcogen analogues
P-65.7.5 Diacyl derivatives of trioxidane and chalcogen analogues
P-65.7.6 Di- and polyanhydrides
P-65.7.7 Cyclic anhydrides
P-65.7.8 Polyfunctional anhydrides

P-65.7.0 Introduction

Anhydrides are compounds consisting of two acyl groups bonded to the same oxygen atom, i.e., acyl-O-acyl. Symmetric and mixed anhydrides have identical and different acyl groups, respectively. The central oxygen atom can be replaced by chalcogen atoms or a peroxy group and its chalcogen analogues.

Polyanhydrides and polyfunctional anhydrides are also described in this Section.

P-65.7.1 Symmetric anhydrides

Symmetric anhydrides of monobasic acids, substituted or unsubstituted, are named by replacing the term 'acid' of an acid name by the class name 'anhydride'.

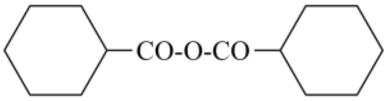
Examples:

CH_3-CO-O-CO-CH_3
acetic anhydride (PIN)

C_6H_5-CS-O-CS-C_6H_5
benzenecarbothioic anhydride (PIN)
thiobenzoic anhydride

(CH_3-CH_2-CH_2-CH_2-CH_2-CO)$_2$O
hexanoic anhydride (PIN)

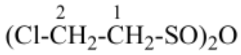
CH_3-CH_2-CS-O-CS-CH_2-CH_3
propanethioic anhydride (PIN)



cyclohexanecarboxylic anhydride (PIN)

C_6H_5-SO_2-O-SO_2-C_6H_5
benzenesulfonic anhydride (PIN)

(Cl-CH_2-CO)$_2$O
chloroacetic anhydride (PIN)



$(\text{Cl-}\overset{2}{C}H_2\text{-}\overset{1}{C}H_2\text{-SO})_2O$

2-chloroethane-1-sulfinic anhydride (PIN)

P-65.7.2 Mixed anhydrides

Anhydrides derived from different monobasic acids are named by citing in alphabetical order the names of the two acids, substituted or unsubstituted, without the class name 'acid' followed by the class name 'anhydride' as a separate word.

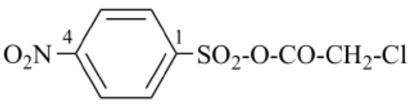
Examples:

CH_3-CO-O-CO-CH_2-CH_3
acetic propanoic anhydride (PIN)

C_6H_5-SO-O-SO_2-CH_2-CH_3
benzenesulfinic ethanesulfonic anhydride (PIN)

C_6H_5-CO-O-CS-CH_3
benzoic ethanethioic anhydride (PIN)
benzoic thioacetic anhydride

CH_3-CO-O-CO-CH_2-Cl
acetic chloroacetic anhydride (PIN)



chloroacetic 4-nitrobenzene-1-sulfonic anhydride (PIN)

Mixed anhydrides with carbonic acid, cyanic acid, and inorganic acids are named as anhydrides. Terms such as 'monoanhydride' are used with di-, tri-, or tetrabasic acids to specify the appropriate number of anhydride linkages.

Examples:

CH_3-CO-O-CN
acetic cyanic anhydride (PIN)

C_6H_5-CO-O-PH_2
benzoic phosphinous anhydride (PIN)

$(HO)_2B$-O-CO-CH_3
acetic boric monoanhydride (PIN)

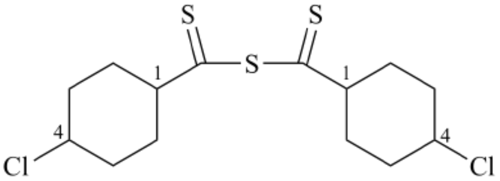
P-65.7.3 Thioanhydrides and other chalcogen analogues

Chalcogen analogues of anhydrides having the general structure –CO-X-CO–, –CO-X-CS–, or –CS-X-CS–, where X is –S –, –Se –, or –Te–, are named using the class names ‘thioanhydride’, ‘selenoanhydride’, or ‘telluroanhydride’, respectively.

Examples:

C_6H_5-CO-S-CO-C_6H_5
benzoic thioanhydride (PIN)

CH_3-CH_2-SO_2-S-CS-C_6H_5
benzenecarbothioic ethanesulfonic thioanhydride (PIN)
ethanesulfonic thiobenzoic thioanhydride



4-chlorocyclohexane-1-carbothioic thioanhydride (PIN)

CH_3-CO-Se-CO-CH_3
acetic selenoanhydride (PIN)

The various unsymmetrical thioanhydrides derived from acetic propanoic anhydride are named as follows.

Examples:

CH_3-CO-O-CO-CH_2-CH_3
acetic propanoic anhydride (PIN)
acetic propionic anhydride

CH_3-CO-O-CS-CH_2-CH_3
acetic propanethioic anhydride (PIN)
acetic thiopropionic anhydride

CH_3-CO-S-CO-CH_2-CH_3
acetic propanoic thioanhydride (PIN)
acetic propionic thioanhydride

CH_3-CS-O-CO-CH_2-CH_3
ethanethioic propanoic anhydride (PIN)
propionic thioacetic anhydride

CH_3-CS-O-CS-CH_2-CH_3
ethanethioic propanethioic anhydride (PIN)
thioacetic thiopropionic anhydride

CH_3-CS-S-CS-CH_2-CH_3
ethanethioic propanethioic thioanhydride (PIN)
thioacetic thiopropionic thioanhydride

CH_3-CH_2-CS-Se-CO-CH_3
acetic propanethioic selenoanhydride (PIN)
acetic thiopropionic selenoanhydride

CH_3-CS-S-CO-CH_2-CH_3
ethanethioic propanoic thioanhydride (PIN)
propionic thioacetic thioanhydride

P-65.7.4 Peroxyanhydrides and chalcogen analogues

Peroxyanhydrides, R-CO-OO-CO-R or R-CO-OO-COR′, are named by replacing the term ‘acid’ of an acid or two different acids by the class name ‘peroxyanhydride’.

Example:

$\mathrm{CH_3\text{-}CO\text{-}OO\text{-}CO\text{-}CH_3}$
acetic peroxyanhydride (PIN)

Related anhydrides, in which the junction between two acyl groups is of the type –SS–, –OS–, –SSe–, etc. are named as ‘dithioperoxyanhydrides’, ‘thioperoxyanhydrides’, ‘selenothioperoxyanhydrides’, etc. When it is necessary to specify the position of the chalcogen atoms between two unsymmetrically substituted acyl groups or two different acyl groups, the acyl group name is preceded by the appropriate italicized capital element symbols indicating its attachment.

Examples:

$\mathrm{CH_3\text{-}CO\text{-}S\text{-}O\text{-}CO\text{-}CH_3}$
acetic thioperoxyanhydride (PIN)

$\mathrm{CH_3\text{-}CO\text{-}S\text{-}O\text{-}CO\text{-}CH_2\text{-}CH_3}$
S-acetic *O*-propanoic thioperoxyanhydride (PIN)

$\mathrm{CH_3\text{-}CO\text{-}SS\text{-}CO\text{-}CH_3}$
acetic dithioperoxyanhydride (PIN)

P-65.7.5 Diacyl derivatives of trioxidane and chalcogen analogues

P-65.7.5.1 Anhydrides derived from peroxy acids and their chalcogen analogues are named substitutively as pseudoketones (see P-64.3). Multiplicative names are preferred when the conditions for their use are fulfilled (see P-15.3).

Examples:

$\mathrm{CH_3\text{-}\overset{1'}{C}O\text{-}OOO\text{-}\overset{1}{C}O\text{-}CH_3}$
1,1′-trioxidanediyldi(ethan-1-one) (PIN)

$\mathrm{CH_3\text{-}CO\text{-}SSSS\text{-}\overset{1}{C}O\text{-}\overset{2}{C}H_2\text{-}\overset{3}{C}H_3}$
1-(acetyltetrasulfanyl)propan-1-one (PIN)

$\mathrm{CH_3\text{-}CO\text{-}S\text{-}O\text{-}S\text{-}CO\text{-}CH_3}$
1,1′-dithioxanediyldi(ethan-1-one) (PIN)

$\mathrm{CH_3\text{-}CO\text{-}OO\text{-}S\text{-}CO\text{-}CH_3}$
1-[(acetylperoxy)sulfanyl]ethan-1-one (PIN)
{not 1-[(acetylsulfanyl)peroxy]ethan-1-one;
the PIN has the lower alphanumerical order}

P-65.7.5.2 Diacyl derivatives of multiatomic chalcogen chains are named by skeletal replacement (‘a’) nomenclature when the conditions for its use are fulfilled (see P-15.4 and P-51.3.1).

Example:

$\mathrm{\overset{1}{C}H_3\text{-}\overset{2}{C}O\text{-}\overset{3}{O}\text{-}\overset{4}{Te}\text{-}\overset{5}{Se}\text{-}\overset{6}{S}\text{-}\overset{7}{C}O\text{-}\overset{8}{C}H_3}$
3-oxa-6-thia-5-selena-4-telluraoctane-2,7-dione (PIN)

P-65.7.6 Di- and polyanhydrides

Di- and polyanhydrides have two or more –CO-O-CO– or related groups, such as $\mathrm{–SO_2\text{-}O\text{-}SO_2–}$, respectively. They are named using the class name ‘dianhydride’, ‘trianhydride’, etc., preceded by the names of the acid groups cited as separate words.

P-65.7.6.1 Dianhydrides are named by citing the acid groups in their order of occurrence in the structure beginning with the end acid group lower in alphabetical order followed by the class term ‘dianhydride’. The numerical prefix ‘di-’ is used to generate preferred IUPAC names.

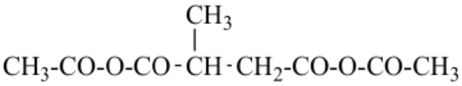
Examples:

$\mathrm{HO{-}B(O\text{-}CO\text{-}CH_3)_2}$
bis(acetyloxy)borinic acid (PIN;
acid is senior to anhydride)
acetic boric dianhydride

CH_3-CO-O-CO-CH_2-CH_2-CO-O-CO-CH_3
diacetic butanedioic dianhydride (PIN)

CH_3-CO-O-SO_2-CH_2-SO_2-O-CO-CH_2-CH_3
acetic methanedisulfonic propanoic dianhydride (PIN)

CH_3-CH_2-CO-O-CO-CH_2-CH_2-CO-O-CO-CH_2-CH_2-CH_3
butanoic butanedioic propanoic dianhydride (PIN)



$$CH_3\text{-}CO\text{-}O\text{-}CO\text{-}\overset{CH_3}{\overset{|}{CH}}\text{-}CH_2\text{-}CO\text{-}O\text{-}CO\text{-}CH_3$$

diacetic 2-methylbutanedioic dianhydride (PIN)

P-65.7.6.2 Linear polyanhydrides are named by one of the following methods:

(1) by selecting the preferred dicarboxylic acid and citing the adjoining acid groups one of which will be substituted using the principles of substitutive nomenclature;

(2) by citing the acid groups, in their order of appearance, in the structure beginning with the end acid group lower in alphabetical order followed by a class term 'dianhydride', 'trianhydride', etc. Numerical prefixes are in preferred IUPAC names.

When there is a choice the second acid group will be the acid group lower in alphabetical order.

Method (1) generates preferred IUPAC names.

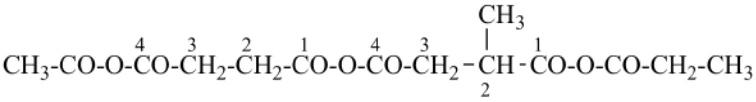
Examples:

CH_3-CO-O-CO-CH_2-CH_2-CO-O-CO-CH_2-CH_2-CO-O-CO-CH_2-CH_3
(1) acetic butanedioic 4-(propanoyloxy)-4-oxobutanoic dianhydride (PIN)
(2) acetic dibutanedioic propanoic trianhydride

CH_3-CO-O-CO-CH_2-CO-O-CO-CH_2-CH_2-CO-O-CO-CH_3
(1) acetic 3-(acetyloxy)-3-oxopropanoic butanedioic dianhydride (PIN)
(2) acetic butanedioic propanedioic acetic trianhydride

When the dibasic acid is substituted, locants are used to locate the terminal acid groups.

Examples:



$$CH_3\text{-}CO\text{-}O\text{-}\overset{4}{C}O\text{-}\overset{3}{C}H_2\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}O\text{-}O\text{-}\overset{4}{C}O\text{-}\overset{3}{C}H_2\text{-}\underset{2}{\overset{CH_3}{\overset{|}{C}}}H\text{-}\overset{1}{C}O\text{-}O\text{-}CO\text{-}CH_2\text{-}CH_3$$

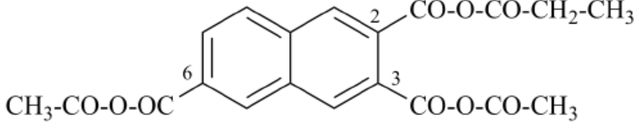
4-[4-(acetyloxy)-4-oxobutanoic] 2-methylbutanedioic 1-propanoic dianhydride (PIN)
4-(acetic butanedioic) 2-methylbutanedioic 1-propanoic trianhydride

$$CH_3\text{-}CO\text{-}O\text{-}\overset{1}{C}O\text{-}\overset{2}{C}H_2\text{-}\overset{3}{C}H_2\text{-}\overset{4}{C}O\text{-}O\text{-}SO_2\text{-}CH_2\text{-}SO_2\text{-}O\text{-}CO\text{-}CH_3$$

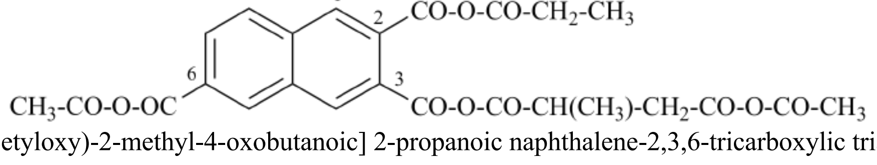
acetic butanedioic [(acetyloxy)sulfonyl]methanesulfonic dianhydride (PIN)
acetic butanedioic methanedisulfonic acetic trianhydride

P-65.7.6.3 Polyanhydrides consisting of a polybasic acid residue and the equivalent number of monobasic residues are named by citing the monobasic acid groups, which may be substituted by additional anhydride linkages, in alphabetical order followed by the polybasic acid residue and the class name 'anhydride' with the appropriate numerical prefix. Locants may be used to specify the positions of the anhydride linkages.

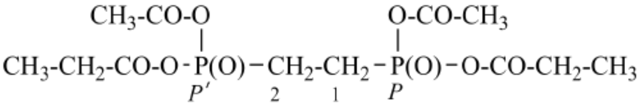
Examples:



3,6-diacetic 2-propanoic naphthalene-2,3,6-tricarboxylic trianhydride (PIN)

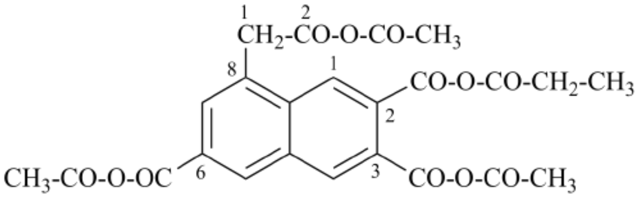


6-acetic 3-[4-(acetyloxy)-2-methyl-4-oxobutanoic] 2-propanoic naphthalene-2,3,6-tricarboxylic trianhydride (PIN)

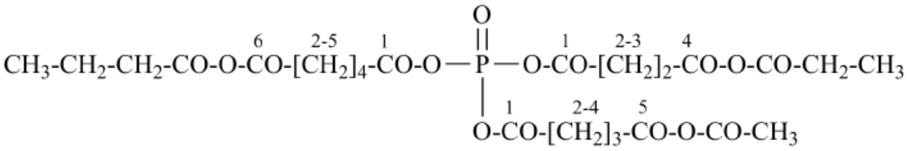


$$\mathrm{CH_3\text{-}CH_2\text{-}CO\text{-}O\text{-}\underset{P'}{\overset{\overset{CH_3\text{-}CO\text{-}O}{|}}{P(O)}}-\underset{2}{CH_2}\text{-}\underset{1}{CH_2}-\underset{P}{\overset{\overset{O\text{-}CO\text{-}CH_3}{|}}{P(O)}}-O\text{-}CO\text{-}CH_2\text{-}CH_3}$$

P,*P*′-diacetic *P*,*P*′-dipropanoic (ethane-1,2-diyl)bis(phosphonic) tetraanhydride (PIN)



3,6-diacetic 2-propanoic 8-[2-(acetyloxy)-2-oxoethyl]naphthalene-2,3,6-tricarboxylic trianhydride (PIN)



$$\mathrm{CH_3\text{-}CH_2\text{-}CH_2\text{-}CO\text{-}O\text{-}\overset{6}{C}O\text{-}\overset{2\text{-}5}{[CH_2]_4}\text{-}\overset{1}{C}O\text{-}O-\underset{\underset{O\text{-}\overset{1}{C}O\text{-}\overset{2\text{-}4}{[CH_2]_3}\text{-}\overset{5}{C}O\text{-}O\text{-}CO\text{-}CH_3}{|}}{\overset{\overset{O}{||}}{P}}-O\text{-}\overset{1}{C}O\text{-}\overset{2\text{-}3}{[CH_2]_2}\text{-}\overset{4}{C}O\text{-}O\text{-}CO\text{-}CH_2\text{-}CH_3}$$

5-(acetyloxy)-5-oxopentanoic 6-(butanoyloxy)-6-oxohexanoic 4-oxo-4-(propanoyloxy)butanoic phosphoric trianhydride (PIN)

P-65.7.6.4 Chalcogen analogues of di- and polyanhydrides

When chalcogen atoms are present in di- and polyanhydrides, their names are formed in different ways.

P-65.7.6.4.1 When all anhydride linkages are identical, as in –CO-S-CO–, names are formed using class names such as ‘thioanhydride’ preceded by the multiplicative prefixes ‘bis-’, ‘tris-’, etc.

Examples:

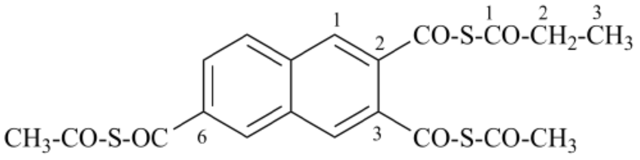
$\mathrm{CH_3\text{-}CO\text{-}S\text{-}CO\text{-}CH_2\text{-}CH_2\text{-}CO\text{-}S\text{-}CO\text{-}CH_3}$
diacetic butanedioic bis(thioanhydride) (PIN)

$\mathrm{CH_3\text{-}CO\text{-}S\text{-}SO_2\text{-}CH_2\text{-}SO_2\text{-}S\text{-}CO\text{-}CH_3}$
diacetic methanedisulfonic bis(thioanhydride) (PIN)

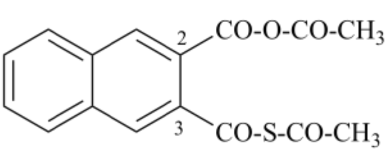
P-65.7.6.4.2 When different chalcogen atoms are present in the anhydride linkages, the usual order of seniority established for chalcogen atoms, O > S > Se > Te, is used to choose the senior anhydride. The senior anhydride chosen as the basis for the name can be an anhydride (see P-65.7.1 through P-65.7.5) or a di- or polyanhydride. Other anhydride linkages are named substitutively.

Examples:

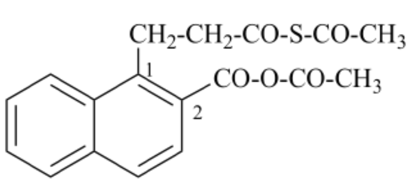
$\mathrm{CH_3\text{-}CO\text{-}O\text{-}CO\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}CO\text{-}S\text{-}CO\text{-}CH_3}$
acetic 5-(acetylsulfanyl)-5-oxopentanoic anhydride (PIN)



3,6-diacetic 2-propanoic naphthalene-2,3,6-tricarboxylic tris(thioanhydride) (PIN)



acetic 3-[(acetylsulfanyl)carbonyl]naphthalene-2-carboxylic anhydride (PIN)



acetic 1-[3-(acetylsulfanyl)-3-oxopropyl]naphthalene-2-carboxylic anhydride (PIN)

P-65.7.6.4.3 When the chalcogen atom replaces an oxygen atom in a carbonyl group, i.e. >C=S, thiocarboxylic acids and thioacyl groups are used in the manner described for anhydrides and polyanhydrides.

Examples:

$CH_3-CS-O-CO-CH_2-CH_2-CO-O-CO-CH_3$
acetic butanedioic ethanethioic dianhydride (PIN)

$CH_3-CO-O-CS-CH_2-CH_2-CS-O-CO-CH_3$
diacetic butanebis(thioic) dianhydride (PIN)

$CH_3-CO-O-CS-CH_2-CH_2-CS-S-CS-CH_3$
acetic 4-[(ethanethioyl)sulfanyl]-4-sulfanylidenebutanethioic anhydride (PIN)

$CH_3-CO-O-CO-CH_2-CH_2-CO-O-CO-CH_2-CH_2-CO-S-CO-CH_2-CH_3$
acetic butanedioic 4-oxo-4-(propanoylsulfanyl)butanoic dianhydride (PIN)

P-65.7.7 Cyclic anhydrides

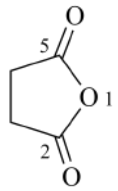
P-65.7.7.1 Cyclic anhydrides formed from two acid groups attached to the same parent hydride structure are named in two ways:

(1) as heterocyclic pseudoketones;

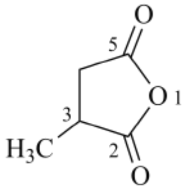
(2) by changing the class term ‘acid’ to ‘anhydride’ in the systematic or retained name of the dibasic acid.

Method (1) generates preferred IUPAC names

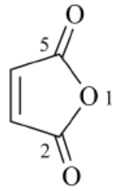
Examples:



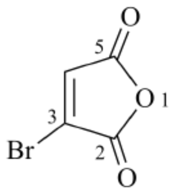
oxolane-2,5-dione (PIN)
3,4-dihydrofuran-2,5-dione
butanedioic anhydride
succinic anhydride



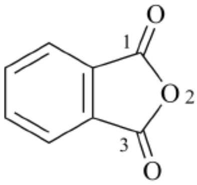
3-methyloxolane-2,5-dione (PIN)
3-methyl-3,4-dihydrofuran-2,5-dione
2-methylbutanedioic anhydride
methylsuccinic anhydride



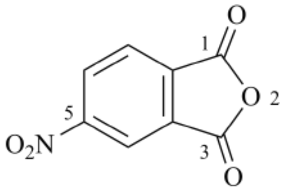
furan-2,5-dione (PIN)
maleic anhydride



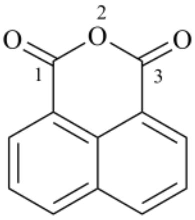
3-bromofuran-2,5-dione (PIN)
bromomaleic anhydride



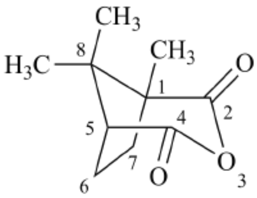
2-benzofuran-1,3-dione (PIN)
isobenzofuran-1,3-dione
phthalic anhydride



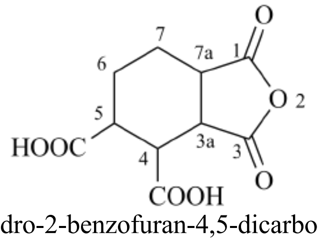
5-nitro-2-benzofuran-1,3-dione (PIN)
5-nitroisobenzofuran-1,3-dione
4-nitrophthalic anhydride



1*H*,3*H*-benzo[*de*][2]benzopyran-1,3-dione (PIN)
1*H*,3*H*-benzo[*de*]isochromene-1,3-dione
naphthalene-1,8-dicarboxylic anhydride



1,8,8-trimethyl-3-oxabicyclo[3.2.1]octane-2,4-dione (PIN)
(also known as camphoric anhydride)



1,3-dioxooctahydro-2-benzofuran-4,5-dicarboxylic acid (PIN)
1,3-dioxooctahydroisobenzofuran-4,5-dicarboxylic acid
cyclohexane-1,2,3,4-tetracarboxylic acid 3,4-anhydride

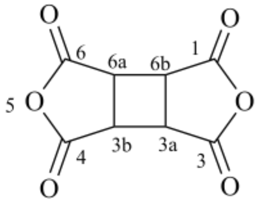
P-65.7.7.2 Cyclic dianhydrides formed from four acid groups attached to the same parent hydride structure are named in two ways:

(1) as heterocyclic pseudoketones;

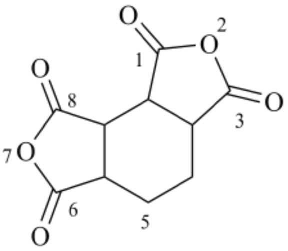
(2) by changing the class term ‘acid’ to ‘dianhydride’ in the systematic or retained name of the tetrabasic acid; the locants of the pair of acid groups are separated by a semicolon.

Method (1) generates preferred IUPAC names

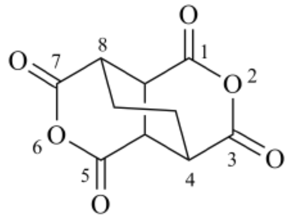
Examples:



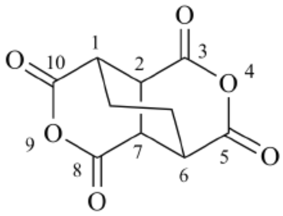
tetrahydrocyclobuta[1,2-*c*:3,4-*c*′]difuran-1,3,4,6-tetrone (PIN)
cyclobutane-1,2,3,4-tetracarboxylic 1,2:3,4-dianhydride



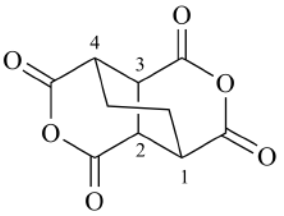
hexahydrobenzo[1,2-*c*:3,4-*c*′]difuran-1,3,6,8-tetrone (PIN)
cyclohexane-1,2,3,4-tetracarboxylic 1,2:3,4-dianhydride



(**I**)



(**II**)



(**III**)

tetrahydro-4,8-ethanopyrano[4,3-*c*]pyran-1,3,5,7-tetrone (PIN) [numbering shown in (**I**)]
{not 4,9-dioxatricyclo[4.4.2.$0^{2,7}$]dodecane-3,5,8,10-tetrone [numbering shown in (**II**)]}
cyclohexane-1,2,3,4-tetracarboxylic 1,3:2,4-dianhydride [numbering shown in (**III**)]

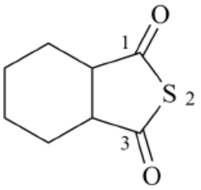
P-65.7.7.3 Chalcogen analogues of cyclic anhydrides are named:

(1) as heterocyclic pseudoketones;

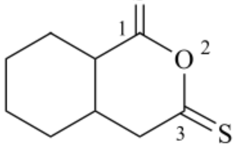
(2) by changing the class term ‘acid’ to ‘dianhydride’ or ‘thioanhydride’, ‘bis(thioanhydride)’, etc., in the systematic or retained name of the dibasic or tetrabasic acid.

Method (1) leads to the preferred IUPAC name.

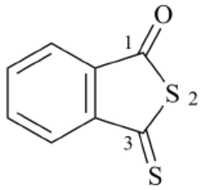
Examples:



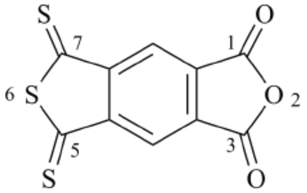
(1) hexahydro-2-benzothiophene-1,3-dione (PIN)
hexahydrobenzo[*c*]thiophene-1,3-dione (PIN)
(2) cyclohexane-1,2-dicarboxylic thioanhydride
hexahydrophthalic thioanhydride



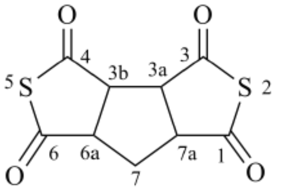
(1) hexahydro-1*H*-2-benzopyran-1,3(4*H*)-dithione (PIN)



(1) 3-sulfanylidene-2-benzothiophen-1-one (PIN)
3-sulfanylidenebenzo[*c*]thiophen-1-one



(1) 5,7-bis(sulfanylidene)-5,7-dihydro-1*H*,3*H*-thieno[3,4-*f*][2]benzofuran-1,3-dione (PIN)
5,7-dithioxo-5,7-dihydro-1*H*,3*H*-thieno[3,4-*f*]isobenzofuran-1,3-dione
(2) 1,3-bis(sulfanylidene)-1,3-dihydro-2-benzothiophene-5,6-dicarboxylic anhydride
1,3-dithioxo-1,3-dihydroisobenzothiophene-5,6-dicarboxylic anhydride



(1) tetrahydro-1*H*-cyclopenta[1,2-*c*:3,4-*c*′]dithiophene-1,3,4,6(3a*H*)-tetrone (PIN)
(2) cyclopentane-1,2,3,4-tetracaboxylic 1,2:3,4-bis(thioanhydride)

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Division VIII Chemical Nomenclature and Structure Representation Division

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Chapter P-6 APPLICATIONS TO SPECIFIC CLASSES OF COMPOUNDS (continued)

(P-66 to P-69)
(continued from P-60 to P-65)

P-60 Introduction
P-61 Substitutive nomenclature: prefix mode
P-62 Amines and imines
P-63 Hydroxy compounds, ethers, peroxols, peroxides and chalcogen analogues
P-64 Ketones, pseudoketones and heterones, and chalcogen analogues
P-65 Acids and derivatives
P-66 Amides, hydrazides, nitriles, aldehydes
P-67 Oxoacids used as parents for organic compounds
P-68 Nomenclature of other classes of compounds
P-69 Organometallic compounds

P-66 AMIDES, IMIDES, HYDRAZIDES, NITRILES, AND ALDEHYDES

P-66.0 Introduction
P-66.1 Amides
P-66.2 Imides
P-66.3 Hydrazides
P-66.4 Amidines, amidrazones, hydrazidines, and amidoximes (amide oximes)
P-66.5 Nitriles
P-66.6 Aldehydes

P-66.0 INTRODUCTION

The classes dealt with in this Section have in common the fact that their retained names are derived from those of acids by changing the ‘ic acid’ ending to a class name, for example ‘amide’, ‘ohydrazide’, ‘nitrile’, or ‘aldehyde’. Their systematic names are formed substitutively by the suffix mode using one of two types of suffix, one that includes the carbon atom, for example, ‘carbonitrile’ for –CN, and one that does not, for example, ‘-nitrile’ for –(C)N. Amidines are named as amides, hydrazidines as hydrazides, and amidrazones as amides or hydrazides.

P-66.1 AMIDES

P-66.1.0 Introduction
P-66.1.1 Primary amides
P-66.1.2 Secondary and tertiary amides
P-66.1.3 ‘Hidden’ amides
P-66.1.4 Chalcogen analogues of amides
P-66.1.5 Lactams, lactims, sultams, and sultims
P-66.1.6 Amides derived from carbonic, cyanic, and the di- and polycarbonic acids
P-66.1.7 Polyfunctional amides

P-66.1.0 Introduction

Amides are derivatives of organic oxoacids in which each hydroxy group has been replaced by an amino or substituted amino group. Chalcogen replacement analogues are called thio-, seleno-, and telluroamides. Compounds having one, two, or three acyl groups on a single nitrogen atom are generically included.

P-66.1.1 Primary amides

P-66.1.1.1 Carboxamides
P-66.1.1.2 Sulfonamides, sulfinamides, and related selenium and tellurium amides
P-66.1.1.3 Substitution of primary amides
P-66.1.1.4 Amides denoted as prefixes

P-66.1.1.1 Carboxamides

Names of carboxamides are formed in two ways:

P-66.1.1.1.1 Substitutive nomenclature
P-66.1.1.1.2 Modification of retained names for acids

P-66.1.1.1.1 Amide names formed by substitutive nomenclature

P-66.1.1.1.1.1 Alicyclic mono- and diamides are named substitutively by adding the suffix ‘amide’, to the appropriate parent hydride name, with elision of the final letter ‘e’ before ‘a’. The multiplying prefix ‘di’ is used to name diamides.

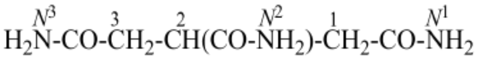
Examples:

$CH_3\text{-}[CH_2]_4\text{-}CO\text{-}NH_2$
hexanamide (PIN)

$H_2N\text{-}CO\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}CO\text{-}NH_2$
pentanediamide (PIN)

P-66.1.1.1.1.2 If an unbranched chain is directly linked to more than two –CO-NH$_2$ groups, these groups are named from the parent hydride by substitutive use of the suffix ‘carboxamide’.

Example:



$$H_2\overset{N^3}{N}\text{-}CO\text{-}\overset{3}{C}H_2\text{-}\overset{2}{C}H(CO\text{-}\overset{N^2}{N}H_2)\text{-}\overset{1}{C}H_2\text{-}CO\text{-}\overset{N^1}{N}H_2$$

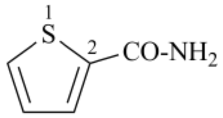
propane-1,2,3-tricarboxamide (PIN)

P-66.1.1.1.1.3 The suffix ‘carboxamide’ is always used to name amides with the –CO-NH$_2$ group attached to a ring, ring system, or to a heteroacyclic parent.

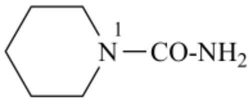
Examples:

$H_2P\text{-}CO\text{-}NH_2$
phosphanecarboxamide (PIN)

$H_2N\text{-}NH\text{-}CO\text{-}NH_2$
hydrazinecarboxamide (PIN)



thiophene-2-carboxamide (PIN)



piperidine-1-carboxamide (PIN)

P-66.1.1.1.2 Amide names formed by modifying retained names of acids

Names of amides derived from carboxylic acids listed in P-65.1.1 are formed by changing the ‘ic acid’ or ‘-oic acid’ ending of the retained names of carboxylic acids into ‘amide’. Names of amides formed by this method are either preferred IUPAC names or names for use in general nomenclature according to the status of the corresponding acid; structures can be substituted in the same way as indicated for the corresponding acids (see P-65.1.1).

P-66.1.1.1.2.1 Only the following four retained names are preferred IUPAC names and can be substituted. The name ‘oxamide’ is a contracted name from ‘oxalamide’ and substitution on the nitrogen atoms is allowed.

$CH_3\text{-}CO\text{-}NH_2$
acetamide (PIN)

$C_6H_5\text{-}CO\text{-}NH_2$
benzamide (PIN)

$H_2N\text{-}CO\text{-}CO\text{-}NH_2$
oxamide (PIN)

$NC\text{-}NH_2$
cyanamide
(PIN, see P-66.1.6.2)

P-66.1.1.1.2.2 The traditional name 'formamide' is retained for $HCO-NH_2$ and is the preferred IUPAC name. Substitution is permitted on the $-NH_2$ group. Substitution of the aldehydic hydrogen is subject to limitations (see P-65.1.8).

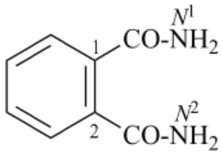
Examples:

$HCO-NH_2$
formamide (PIN)

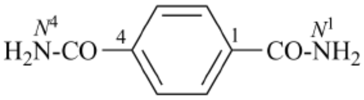
$Cl-CO-NH_2$
carbonochloridic amide (PIN)
(not 1-chloroformamide)

P-66.1.1.1.2.3 For general nomenclature only, the names furanamide, phthalamide, isophthalamide, and terephthalamide are retained with substitution allowed (see P-65.1.1.2.1). Systematic names formed according to P-65.1.2 are the preferred IUPAC names.

Examples:



benzene-1,2-dicarboxamide (PIN)
phthalamide



benzene-1,4-dicarboxamide (PIN)
terephthalamide

P-66.1.1.1.2.4 Amides derived from retained acid names given in P-65.1.1.2 are only used in general nomenclature; no substitution is allowed, even on amide nitrogen atoms. Preferred IUPAC names are systematic names as given by P-65.1.2.

Examples:

$\overset{3}{C}H_2=\overset{2}{C}H-\overset{1}{C}O-NH_2$
prop-2-enamide (PIN)
acrylamide

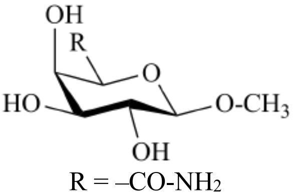
$\overset{3}{C}H_2=\overset{2}{C}H-\overset{1}{C}O-NH-CH_3$
N-methylprop-2-enamide (PIN)
(not *N*-methylacrylamide;
substitution is not allowed on acrylamide)

$\overset{3}{C}H_3-\overset{2}{C}H(OH)-\overset{1}{C}O-NH_2$
2-hydroxypropanamide (PIN)
lactamide

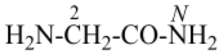
$\overset{3}{C}H_3-\overset{2}{C}H(OH)-\overset{1}{C}O-NH-CH_3$
2-hydroxy-*N*-methylpropanamide (PIN)
(not *N*-methyllactamide)

P-66.1.1.1.2.5 Names for amides derived from carbohydrate acids and α-amino acids are discussed in P-102.5.6.6.2.1, P-102.5.6.6.5, and in P-103.2.7, respectively.

Examples:



$R = -CO-NH_2$
methyl β-D-galactopyranosiduronamide



$H_2N\text{-}\overset{2}{C}H_2\text{-}CO\text{-}\overset{N}{N}H_2$

2-aminoacetamide
glycinamide

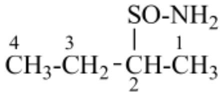
P-66.1.1.2 Sulfonamides, sulfinamides, and related selenium and tellurium amides Sulfonamides, sulfinamides, and the analogous selenium and tellurium amides are named substitutively using the following suffixes:

$–SO_2\text{-}NH_2$	sulfonamide (preselected suffix)
$–SO\text{-}NH_2$	sulfinamide (preselected suffix)
$–SeO_2\text{-}NH_2$	selenonamide (preselected suffix)
$–SeO\text{-}NH_2$	seleninamide (preselected suffix)
$–TeO_2\text{-}NH_2$	telluronamide (preselected suffix)
$–TeO\text{-}NH_2$	tellurinamide (preselected suffix)

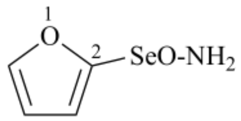
These suffixes may be assigned to any position of a parent hydride.

Examples:

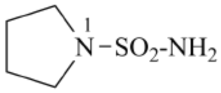
$CH_3\text{-}SO_2\text{-}NH_2$
methanesulfonamide (PIN)



butane-2-sulfinamide (PIN)



furan-2-seleninamide (PIN)



pyrrolidine-1-sulfonamide (PIN)

P-66.1.1.3 Substitution of primary amides

P-66.1.1.3.1 *N*-Substitution
P-66.1.1.3.2 Hydroxamic acids
P-66.1.1.3.3 Amic acids
P-66.1.1.3.4 Anilides
P-66.1.1.3.5 General substitution of amides

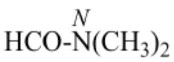
P-66.1.1.3.1 *N*-Substitution

P-66.1.1.3.1.1 Substituted primary amides, with general structures such as R-CO-NHR′ and R-CO-NR′R″, and the corresponding amides derived from chalcogen acids are named by citing the substituents R′ and R″ as prefixes preceded by the locant *N* when one amide group is present. In di- and polyamides, except for geminal diamides, *N* locants with superscripted arabic numbers, which are the locants of the parent structure, are used to differentiate the nitrogen atoms, for example, N^1, N^3, etc. (see also P-62.2.4.1.2). The recommended *N* locants for geminal diamides are discussed in P-66.1.1.3.1.2.

> Superscript arabic numbers are now used to differentiate the nitrogen atoms of diamides, where primes (′), double primes (″), triple primes (‴), etc. were formerly used.

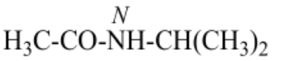
N-Substitution of primary amides is not allowed when amides having retained names are designated as not substitutable.

Examples:



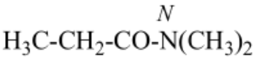
$HCO\text{-}\overset{N}{N}(CH_3)_2$

dimethylformamide (PIN)



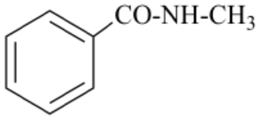
$H_3C\text{-}CO\text{-}\overset{N}{N}H\text{-}CH(CH_3)_2$

N-(propan-2-yl)acetamide (PIN)

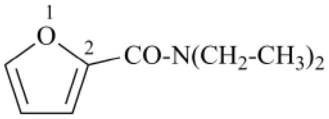


$H_3C\text{-}CH_2\text{-}CO\text{-}\overset{N}{N}(CH_3)_2$

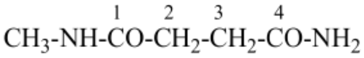
N,*N*-dimethylpropanamide (PIN)
(not *N*,*N*-dimethylpropionamide;
substitution is not allowed on propionamide)



N-methylbenzamide (PIN)

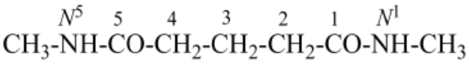


N,*N*-diethylfuran-2-carboxamide (PIN)
N,*N*-diethyl-2-furamide



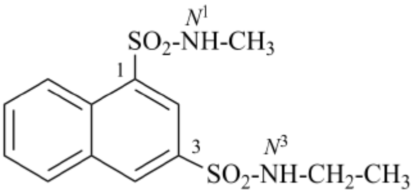
$CH_3\text{-}NH\text{-}\overset{1}{C}O\text{-}\overset{2}{C}H_2\text{-}\overset{3}{C}H_2\text{-}\overset{4}{C}O\text{-}NH_2$

N^1-methylbutanediamide (PIN)



$\overset{N^5}{CH_3\text{-}NH}\text{-}\overset{5}{C}O\text{-}\overset{4}{C}H_2\text{-}\overset{3}{C}H_2\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}O\text{-}\overset{N^1}{NH}\text{-}CH_3$

N^1,*N*^{5}-dimethylpentanediamide (PIN)

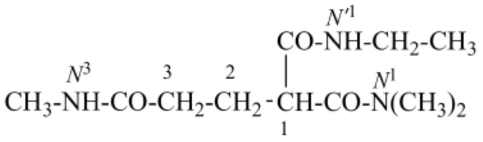


N^3-ethyl-*N*^{1}-methylnaphthalene-1,3-disulfonamide (PIN)

P-66.1.1.3.1.2 Locants for geminal carboxamide groups

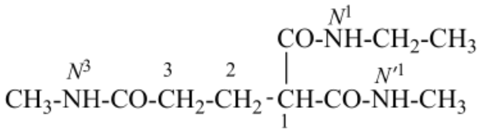
When geminal carboxamide groups are present, the locants *N*, *N*′, etc. are used in association with the numerical locant indicating the position of the groups on a chain or ring. Lowest locants are assigned to the most substituted group; when there is a choice, lowest locants are assigned to the first cited *N*-substituent.

Examples:



$\overset{N^3}{CH_3\text{-}NH}\text{-}\overset{3}{C}O\text{-}\overset{2}{C}H_2\text{-}CH_2\text{-}\underset{1}{\overset{\overset{N'^1}{CO\text{-}NH\text{-}CH_2\text{-}CH_3}}{\overset{|}{C}H}}\text{-}CO\text{-}\overset{N^1}{N}(CH_3)_2$

N′^{1}-ethyl-*N*^{1},*N*^{1},*N*^{3}-trimethylpropane-1,1,3-tricarboxamide (PIN)



$\overset{N^3}{CH_3\text{-}NH}\text{-}\overset{3}{C}O\text{-}\overset{2}{C}H_2\text{-}CH_2\text{-}\underset{1}{\overset{\overset{N^1}{CO\text{-}NH\text{-}CH_2\text{-}CH_3}}{\overset{|}{C}H}}\text{-}CO\text{-}\overset{N'^1}{NH}\text{-}CH_3$

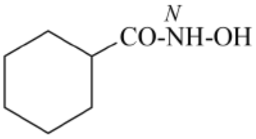
N^1-ethyl-*N*′^{1},*N*^{3}-dimethylpropane-1,1,3-tricarboxamide (PIN)

P-66.1.1.3.2 Hydroxamic acids

Hydroxamic acids have the generic structure R-CO-NH-OH and are named as *N*-hydroxy amides (see P-65.1.3.4). The suffixes ‘hydroxamic acid’ and ‘carbohydroxamic acid’ may be used in general nomenclature.

Examples:

$CH_3\text{-}CH_2\text{-}CO\text{-}NH\text{-}OH$
N-hydroxypropanamide (PIN)
(not propanohydroxamic acid)



N-hydroxycyclohexanecarboxamide (PIN)
(not cyclohexanecarbohydroxamic acid)

P-66.1.1.3.3 Amic acids

Amic acids are derivatives of dicarboxylic acids having a retained name and when one carboxylic group has been changed to a carboxamide group. Preferred IUPAC names for amic acids are generated by method (1) in P-66.1.1.4.1.1. They may also be named by methods (2) and (3) and by replacing the 'ic acid' ending in the retained name by 'amic acid' (see P-65.1.6.1).

Examples:

$\mathrm{H_2N\text{-}\overset{10}{C}O\text{-}[CH_2]_8\text{-}\overset{1}{C}OOH}$

(1) 10-amino-10-oxodecanoic acid (PIN)
(2) 9-carbamoylnonanoic acid
(3) 9-(aminocarbonyl)nonanoic acid

$\mathrm{H_2N\text{-}\overset{3}{C}O\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}OOH}$

(1) 3-amino-3-oxopropanoic acid (PIN)
(2) carbamoylacetic acid
(3) (aminocarbonyl)acetic acid
malonamic acid (see P-65.1.6.1)

P-66.1.1.3.4 Anilides

N-Phenyl derivatives of primary amides are called 'anilides' and may be named using the term 'anilide' in place of 'amide' in systematic or retained names of amides. The locants for substituents in the *N*-phenyl ring of anilides are primed numbers. However, names expressing *N*-substitution by a phenyl group on an amide are preferred IUPAC names.

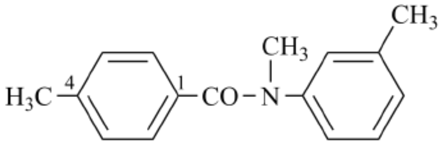
Examples:

$\mathrm{HCO\text{-}NH\text{-}C_6H_5}$
N-phenylformamide (PIN)
formanilide

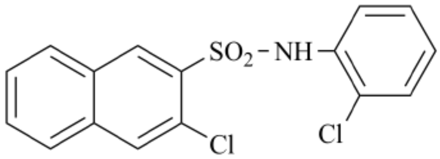
$\mathrm{CH_3\text{-}CO\text{-}NH\text{-}C_6H_5}$
N-phenylacetamide (PIN)
acetanilide

$\mathrm{CH_3\text{-}[CH_2]_4\text{-}CO\text{-}NH\text{-}C_6H_5}$
N-phenylhexanamide (PIN)
hexananilide

$\mathrm{C_6H_5\text{-}CO\text{-}N(CH_3)\text{-}C_6H_5}$
N-methyl-*N*-phenylbenzamide (PIN)
N-methylbenzanilide



N,4-dimethyl-*N*-(3-methylphenyl)benzamide (PIN)
N,3′,4-trimethylbenzanilide



3-chloro-*N*-(2-chlorophenyl)naphthalene-2-sulfonamide (PIN)
2′,3-dichloronaphthalene-2-sulfonanilide

P-66.1.1.3.5 General substitution of amides

Substitution of amides is expressed by prefixes; numerical, *N*, and *N′* locants are used as required. *N*-Substitution of amides follows the substitution rules for carboxylic acids described in P-65.1.2.4.

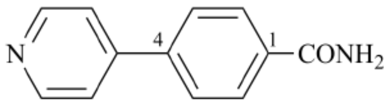
Examples:

$$\text{Cl-}\overset{3}{\text{C}}\text{H}_2\text{-}\overset{2}{\text{C}}\text{H}_2\text{-}\overset{1}{\text{C}}\text{O-NH}_2$$

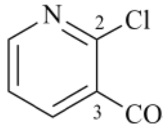
3-chloropropanamide (PIN)
(not 3-chloropropionamide;
no substitution on propionamide)

$$\text{Cl-}\overset{4}{\text{C}}\text{H}_2\text{-}\overset{3}{\text{C}}\text{H}_2\text{-}\overset{2}{\text{C}}\text{H}_2\text{-}\overset{1}{\text{C}}\text{O-N(CH}_3\text{)}_2$$

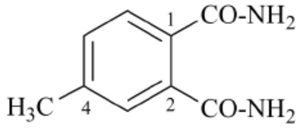
4-chloro-*N*,*N*-dimethylbutanamide (PIN)
(not 4-chloro-*N*,*N*-dimethylbutyramide;
no substitution on butyramide)



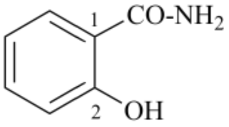
4-(pyridin-4-yl)benzamide (PIN)
4-(4-pyridyl)benzamide



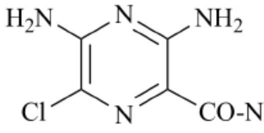
2-chloropyridine-3-carboxamide (PIN)
(not 2-chloronicotinamide)



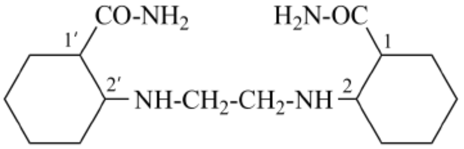
4-methylbenzene-1,2-dicarboxamide (PIN)
4-methylphthalamide



2-hydroxybenzamide (PIN)
(not salicylamide)



3,5-diamino-6-chloropyrazine-2-carboxamide (PIN)



2,2′-[ethane-1,2-diylbis(azanediyl)]di(cyclohexane-1-carboxamide) (PIN)

P-66.1.1.4 Amides denoted as prefixes

Two different substituent groups can be derived from amides and expressed as prefixes in the presence of a characteristic group having seniority for citation as suffix:

P-66.1.1.4.1 Substituents of the types $–\text{CO-NH}_2$ and $–\text{CO-CO-NH}_2$
P-66.1.1.4.2 Substituents of the types $–\text{SO}_2\text{-NH}_2$, $–\text{SO-NH}_2$ and their selenium and tellurium analogues
P-66.1.1.4.3 Substituents of the types –NH-CO-R and $–\text{NH-SO}_2\text{-R}$
P-66.1.1.4.4 Substituent groups R-CO-N< and R-CO-N=, or $\text{R-SO}_2\text{-N<}$ and $\text{R-SO}_2\text{-N=}$ (and selenium and tellurium analogues)
P-66.1.1.4.5 Substituent groups derived from oxamide, $\text{H}_2\text{N-CO-CO-NH}_2$

P-66.1.1.4.1 Substituents of the types $–\text{CO-NH}_2$ and $–\text{CO-CO-NH}_2$.

P-66.1.1.4.1.1 In the presence of a characteristic group having priority for citation as suffix or if all carbamoyl groups cannot be included in the suffix, the –CO-NH$_2$ group is named in three different ways:

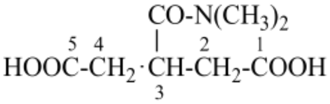
(1) by using the two prefixes ‘amino’ and ‘oxo’ to denote such groups on terminal atoms of carbon chains having more than one carbon atom;

(2) by using the acyl group name ‘carbamoyl’ (see P-65.2.1.5);

(3) by using the prefix ‘aminocarbonyl’.

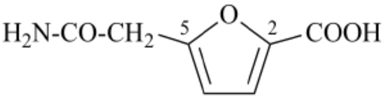
For generation of IUPAC preferred names, method (1) is preferred for chains and method (2) for rings and ring systems, heterogeneous chains, and on nonterminal atoms of carbon chains. Carbamoyl and amino groups may be substituted in the normal way.

Examples:

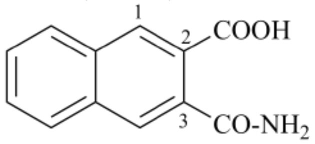


$$\mathrm{HOO\overset{5}{C}\text{-}\overset{4}{C}H_2\cdot\underset{3}{\overset{\overset{\textstyle CO\text{-}N(CH_3)_2}{|}}{C}}H\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}OOH}$$

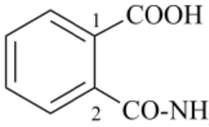
(2) 3-(dimethylcarbamoyl)pentanedioic acid (PIN)
(3) 3-[(dimethylamino)carbonyl]pentanedioic acid



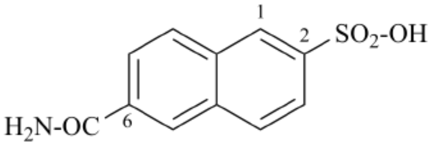
(1) 5-(2-amino-2-oxoethyl)furan-2-carboxylic acid (PIN)
(2) 5-(carbamoylmethyl)furan-2-carboxylic acid
(3) 5-[(aminocarbonyl)methyl]furan-2-carboxylic acid



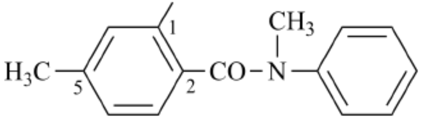
(2) 3-carbamoylnaphthalene-2-carboxylic acid (PIN)
3-carbamoyl-2-naphthoic acid
(3) 3-(aminocarbonyl)naphthalene-2-carboxylic acid
3-(aminocarbonyl)-2-naphthoic acid



(2) 2-carbamoylbenzoic acid (PIN)
(3) 2-(aminocarbonyl)benzoic acid
phthalamic acid (see P-65.1.6.1)



(2) 6-carbamoylnaphthalene-2-sulfonic acid (PIN)
(3) 6-(aminocarbonyl)naphthalene-2-sulfonic acid



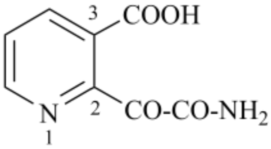
(2) 5-methyl-2-[methyl(phenyl)carbamoyl]benzoic acid (PIN)
(3) 5-methyl-2-[(*N*-methylanilino)carbonyl]benzoic acid
5-methyl-2-{[methyl(phenyl)amino]carbonyl}benzoic acid

P-66.1.1.4.1.2 Similarly, the group –CO-CO-NH$_2$ is named using the prefixes ‘amino’ and ‘oxo’ as in method (1) in P-66.1.1.4.1.1; by using the name ‘oxamoyl’ as in method (2) in P-66.1.1.4.1.1; and by using the prefix ‘aminooxalyl’ as in method (3) in P-66.1.1.4.1.1.

Examples:

$$\mathrm{H_2N\text{-}\overset{4}{C}O\text{-}\overset{3}{C}O\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}OOH}$$

(1) 4-amino-3,4-dioxobutanoic acid (PIN)
(2) oxamoylacetic acid
(3) (aminooxalyl)acetic acid



(2) 2-oxamoylpyridine-3-carboxylic acid (PIN)
(3) 2-(aminooxalyl)pyridine-3-carboxylic acid

P-66.1.1.4.2 Substituents of the types $–SO_2-NH_2$, $–SO-NH_2$, and their selenium and tellurium analogues

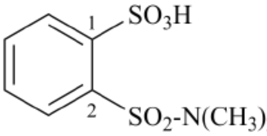
In the presence of a characteristic group having priority for citation as suffix, the groups $–SO_2-NH_2$, $–SO-NH_2$ and related selenium and tellurium groups are named in two ways corresponding to methods (2) and (3) for the $–CO-NH_2$ group above in P-66.1.1.4.1:

(2) by using the acyl group ‘sulfamoyl’ (for sulfonamides only) (see P-65.3.2.3);

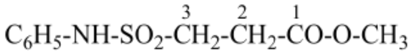
(3) by using the prefixes ‘amino...sulfonyl’, ‘amino...sulfinyl’, ‘amino...selenonyl’, ‘amino...seleninyl’, ‘amino...telluronyl’, or ‘amino...tellurinyl’.

For $–SO_2-NH_2$, method (2) generates preferred IUPAC names; for all other groups method (3) is the only method for generation of preferred IUPAC names.

Examples:

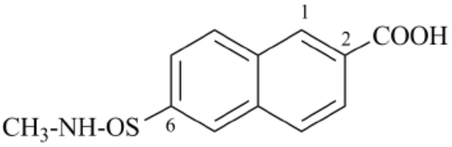


(2) 2-(dimethylsulfamoyl)benzene-1-sulfonic acid (PIN)
(3) 2-[(dimethylamino)sulfonyl]benzene-1-sulfonic acid



$$C_6H_5\text{-}NH\text{-}SO_2\text{-}\overset{3}{C}H_2\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}O\text{-}O\text{-}CH_3$$

methyl 3-(phenylsulfamoyl)propanoate (PIN)
(3) methyl 3-[(phenylamino)sulfonyl]propanoate
methyl 3-(anilinosulfonyl)propanoate



(3) 6-[(methylamino)sulfinyl]naphthalene-2-carboxylic acid (PIN)
(3) 6-[(methylamino)sulfinyl]-2-naphthoic acid,

P-66.1.1.4.3 Substituents of the types $–NH-CO-R$ and $–NH-SO_2-R$

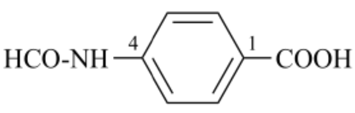
When a group having preference for citation as a principal characteristic group is present, the group R-CO-NH–, or $R-SO_2-NH–$ (and selenium and tellurium analogues) of an *N*-substituted amide is named in two ways:

(1) substitutively, by using a prefix formed by changing the final letter ‘e’ in the complete name of the amide to ‘o’, thus changing the suffixes ‘amide’ and ‘carboxamide’ into ‘amido’ and ‘carboxamido’, respectively, ‘diamide’ to ‘diamido’ or ‘sulfonamide’ to ‘sulfonamido’, etc.;

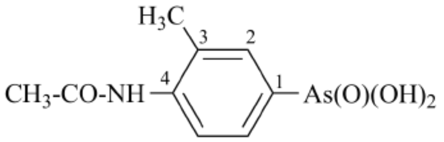
(2) substitutively, by using ‘acylamino’ prefixes formed by substituting the substituent group ‘amino’ with the name of the acyl group.

Method (1) generates preferred IUPAC names.

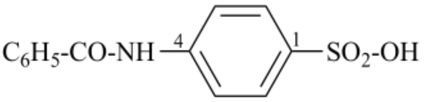
Examples:



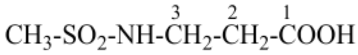
(1) 4-formamidobenzoic acid (PIN)
(2) 4-(formylamino)benzoic acid



(1) (4-acetamido-3-methylphenyl)arsonic acid (PIN)
(2) [4-(acetylamino)-3-methylphenyl]arsonic acid

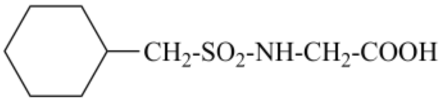


(1) 4-benzamidobenzene-1-sulfonic acid (PIN)
(2) 4-(benzoylamino)benzene-1-sulfonic acid

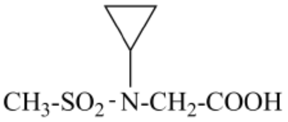


$$CH_3\text{-}SO_2\text{-}NH\text{-}\overset{3}{C}H_2\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}OOH$$

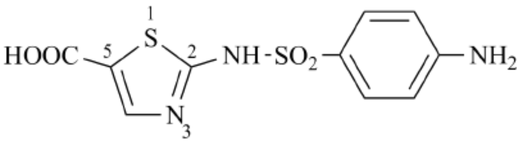
(1) 3-(methanesulfonamido)propanoic acid (PIN)
(2) 3-[(methanesulfonyl)amino]propanoic acid



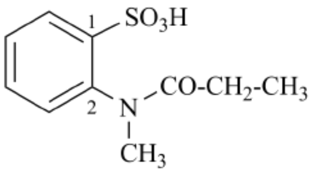
N-(cyclohexylmethanesulfonyl)glycine
(1) (1-cyclohexylmethanesulfonamido)acetic acid
(2) {[(cyclohexylmethyl)sulfonyl]amino}acetic acid



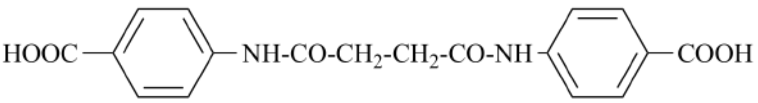
N-cyclopropyl-*N*-(methanesulfonyl)glycine
(1) (*N*-cyclopropylmethanesulfonamido)acetic acid
(2) [(cyclopropyl(methanesulfoyl)amino]acetic acid



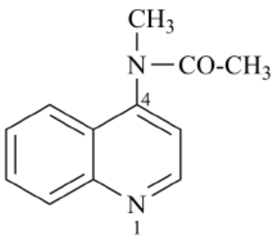
(1) 2-(4-aminobenzene-1-sulfonamido)-1,3-thiazole-5-carboxylic acid (PIN)
(not 2-sulfanilamidothiazole-5-carboxylic acid;
sulfanilic acid is not a retained name)
(2) 2-{[(4-aminophenyl)sulfonyl]amino}-1,3-thiazole-5-carboxylic acid



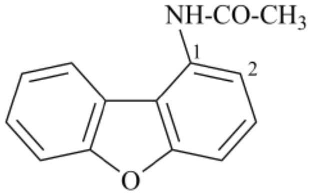
(1) 2-(*N*-methylpropanamido)benzene-1-sulfonic acid (PIN)
(2) 2-[methyl(propanoyl)amino]benzene-1-sulfonic acid



(1) 4,4′-butanediamidodibenzoic acid (PIN)
(2) 4,4′-[butanedioylbis(azanediyl)]dibenzoic acid
4,4′-[1,4-dioxobutane-1,4-diylbis(azanediyl)]dibenzoic acid



N-methyl-*N*-(quinolin-4-yl)acetamide (PIN)
(not 4-(*N*-methylacetamido)quinoline)
{not 4-[acetyl(methyl)amino]quinoline}



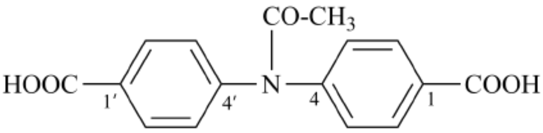
N-(dibenzo[*b*,*d*]furan-1-yl)acetamide (PIN)
(not 1-acetamidodibenzofuran)
[not 1-(acetylamino)dibenzofuran]

> When an amide is the principal function, it must be named as such. The method of considering amides as substituents on polycyclic ring systems, described in the 1993 Recommendations (ref. 2), should be avoided, even in general nomenclature (see also P-66.1.3).

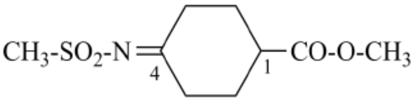
P-66.1.1.4.4 Substituent groups R-CO-N< and R-CO-N=, or R-SO_2-N< and R-SO_2-N= (and selenium and tellurium analogues)

When a group having preference for citation as a principal characteristic group is present, the groups R-CO-N< and R-CO-N=, or R-SO_2-N< and R-SO_2-N= (and selenium and tellurium analogues) of an *N*-substituted amide are named by combining acyl group names with those of the appropriate nitrogen substituent groups, azanediyl and imino, respectively.

Examples:



4,4′-(acetylazanediyl)dibenzoic acid (PIN)



methyl 4-[(methanesulfonyl)imino]cyclohexane-1-carboxylate (PIN)

P-66.1.1.4.5 Substituent groups derived from oxamide, H_2N-CO-CO-NH_2

P-66.1.1.4.5.1 Prefixes for the group H_2N-CO-CO-NH– are ‘oxamoylamino’ (preferred prefix) or ‘amino(oxo)acetamido’. The preferred prefix for the group H_2N-CO-CO-N= is ‘oxamoylimino’.

Example:

H_2N-CO-CO-N=CH-CH_2-COOH
3-(oxamoylimino)propanoic acid (PIN)
3-{[amino(oxo)acetyl]imino}propanoic acid.

P-66.1.1.4.5.2 Prefixes derived from oxamide for use in multiplicative nomenclature

Concatenated preferred prefixes for the groups –HN-CO-CO-NH–, >N-CO-CO-N<, and =N-CO-CO-N= are ‘oxalylbis(azanediyl)’, ‘oxalyldinitrilo’, and ‘oxalylbis(azanylylidene)’, respectively. The preferred prefix for the group H_2N-CO-CO-N< is ‘oxamoylazanediyl,

Example:

NC-CH_2-NH-CO-CO-NH-CH_2-CN
N^1,N^2-bis(cyanomethyl)oxamide (PIN)
(not 2,2′-[oxalylbis(azanediyl)]diacetonitrile)
(not 2,2′-[ethanedioylbis(azanediyl)]diacetonitrile)

P-66.1.2 Secondary and tertiary amides

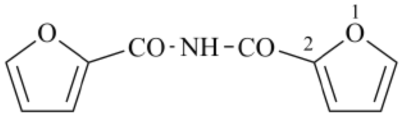
Amides having general formulas $(R\text{-}CO)_2NH$, $(R\text{-}SO_2)_2NH$, etc., and $(R\text{-}CO)_3N$, $(R\text{-}SO_2)_3N$, etc., respectively, are named as *N*-acyl derivatives of the senior primary amide or preferred prefix. Names based on the substitution of the parent hydride ‘azane’ or the pseudo parent hydride ‘amine’ by acyl groups, for example, diacetylazane or diacetylamine, as recommended in the 1993 Recommendations (ref. 2) are not included in these recommendations, nor are trivial names such as diacetamide, triacetamide, dibenzamide, and tribenzamide.

Examples:

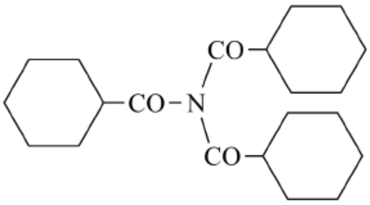
HCO-NH-CHO
N-formylformamide (PIN)
(not diformylazane)
(not diformylamine)
(not diformamide)

$(CH_3\text{-}CO)_2N\text{–}$
N-acetylacetamido (preferred prefix)
diacetylamino
(not diacetylazanyl)
(not diacetamido)

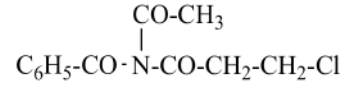
$C_6H_5\text{-}CO\text{-}NH\text{-}CO\text{-}CH_3$
N-acetylbenzamide (PIN)
[not acetyl(benzoyl)azane]
[not acetyl(benzoyl)amine]



N-(furan-2-carbonyl)furan-2-carboxamide (PIN)
[not di(furan-2-carbonyl)azane]
[not di(furan-2-carbonyl)amine]

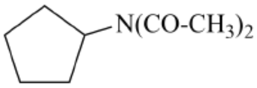


N,*N*-di(cyclohexanecarbonyl)cyclohexanecarboxamide (PIN)
[not tri(cyclohexanecarbonyl)azane]
[not tri(cyclohexanecarbonyl)amine]

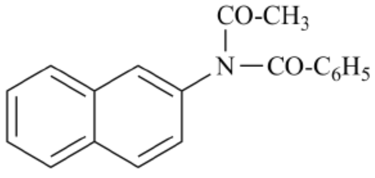


$$C_6H_5\text{-}CO\text{-}N(CO\text{-}CH_3)\text{-}CO\text{-}CH_2\text{-}CH_2\text{-}Cl$$

N-acetyl-*N*-(3-chloropropanoyl)benzamide (PIN)
[not acetyl(benzoyl)(3-chloropropanoyl)azane]
[not acetyl(benzoyl)(3-chloropropanoyl)amine]



N-acetyl-*N*-cyclopentylacetamide (PIN)
[not diacetyl(cyclopentyl)azane]
[not diacetyl(cyclopentyl)amine]



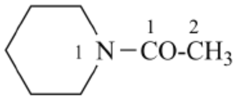
N-acetyl-*N*-(naphthalen-2-yl)benzamide (PIN)
[not acetyl(benzoyl)(naphthalen-2-yl)azane]
[not acetyl(benzoyl)(naphthalen-2-yl)amine]

P-66.1.3 ‘Hidden’ amides

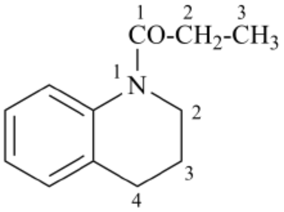
An *N*-acyl group attached to a nitrogen atom of a heterocyclic system has been called a ‘hidden amide’, i.e., an amide that cannot be named as such by accepted substitutive principles. The traditional way to name such compounds by using acyl groups as substituents on the nitrogen atom of the heterocyclic system is allowed but only in general nomenclature. Such compounds are now considered as pseudoketones (see P-64.3) and preferred IUPAC names are constructed accordingly.

An *N*-acyl group attached to a nitrogen atom of a heterocyclic system is now preferably named as a pseudoketone (see P-64.1.2.1, P-64.3) and not as an acyl substituent on the nitrogen as in previous recommendations; the latter method can be used in general nomenclature.

Examples:



1-(piperidin-1-yl)ethan-1-one (PIN)
1-acetylpiperidine



1-(3,4-dihydroquinolin-1(2*H*)-yl)propan-1-one (PIN)
1-propanoyl-1,2,3,4-tetrahydroquinoline
1-propionyl-1,2,3,4-tetrahydroquinoline

P-66.1.4 Chalcogen analogues of amides

Chalcogen analogues of amides are named systematically. Prefixes, such as ‘thio’, modifying retained names are no longer recommended for preferred names.

P-66.1.4.1 Names of chalcogen analogues of primary amides

P-66.1.4.1.1 Names are formed by using suffixes modified by functional replacement nomenclature using prefixes and infixes.

Examples:

–(C)S-NH_2	-thioamide (preferred suffix)
–CS-NH_2	-carbothioamide (preferred suffix)
–S(O)(S)-NH_2	-sulfonothioamide (preselected suffix)
–S(S)(S)-NH_2	-sulfonodithioamide (preselected suffix)
–S(S)-NH_2	-sulfinothioamide (preselected suffix)

For a more extended list, see Table 4.4.

Examples:

HCS-NH_2
methanethioamide (PIN)
thioformamide

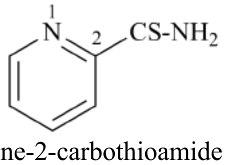
$\text{CH}_3\text{-CS-NH}_2$
ethanethioamide (PIN)
thioacetamide

$\text{C}_6\text{H}_5\text{-CS-NH}_2$
benzenecarbothioamide (PIN)
thiobenzamide

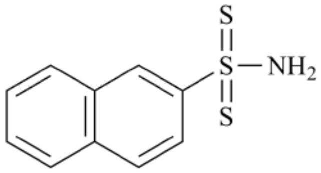
$\text{H}_2\text{N-CS-CH}_2\text{-CH}_2\text{-CS-NH}_2$
butanedithioamide (PIN)

$\text{CH}_3\text{-[CH}_2\text{]}_4\text{-CS-NH}_2$
hexanethioamide (PIN)

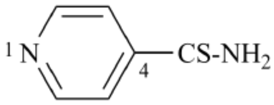
$\text{CH}_3\text{-CH}_2\text{-CS-NH}_2$
propanethioamide (PIN)
(not thiopropionamide)



pyridine-2-carbothioamide (PIN)



naphthalene-2-sulfonodithioamide (PIN)



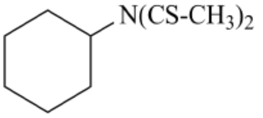
pyridine-4-carbothioamide (PIN)
(not thioisonicotinamide)

P-66.1.4.2 Names for chalcogen analogues of secondary and tertiary amides

Names are formed by the addition of appropriate prefixes to names described in P-65.1.7.2.3

Examples:

$CH_3\text{-}CS\text{-}NH\text{-}CS\text{-}CH_3$
N-(ethanethioyl)ethanethioamide (PIN)
N-(thioacetyl)thioacetamide



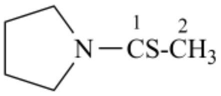
N-cyclohexyl-*N*-(ethanethioyl)ethanethioamide (PIN)
N-cyclohexyl-*N*-(thioacetyl)thioacetamide

$CH_3\text{-}CH_2\text{-}CS\text{-}NH\text{-}CO\text{-}CH_3$
N-(propanethioyl)acetamide (PIN)

P-66.1.4.3 Names of chalcogen derivatives of ‘hidden’ amides

Names are formed as described in P-64.6.1 for chalcogen derivatives of pseudoketones.

Example:



1-(pyrrolidin-1-yl)ethane-1-thione (PIN)
[not 1-(ethanethioyl)pyrrolidine]

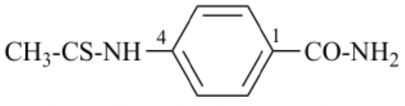
P-66.1.4.4 Names of substituent groups derived from chalcogen derivatives of amides In the presence of a function having priority for citation as suffix, the amide function is expressed in two ways:

(1) by a prefix formed by changing the final letter ‘e’ in the name of the amide into ‘o’;

(2) by the appropriate prefixes, such as amino, in conjunction with sulfanylidene or thioxo, as well as carbonothioyl (not thiocarbonyl) for –CS– or carbamothioyl (not thiocarbamoyl) for $–CS\text{-}NH_2$.

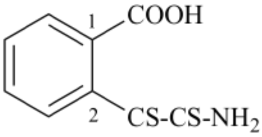
Examples:

$H_2N\text{-}\overset{3}{C}S\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}OOH$
3-amino-3-sulfanylidenepropanoic acid (PIN)
3-amino-3-thioxopropanoic acid
carbamothioylacetic acid
(aminocarbonothioyl)acetic acid



4-(ethanethioamido)benzamide (PIN)
4-[(ethanethioyl)amino]benzamide
4-(thioacetamido)benzamide

$CH_3\text{-}S(S)\text{-}NH\text{-}CH_2\text{-}COOH$
[(methanesulfinothioyl)amino]acetic acid (PIN)



2-[amino(sulfanylidene)ethanethioyl]benzoic acid (PIN)

P-66.1.5 Lactams, lactims, sultams, and sultims

P-66.1.5.1 Lactams and lactims

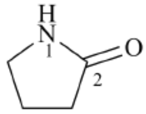
Intramolecular amides of amino carboxylic acids, –CO-NH–, are called ‘lactams’ and their tautomers, –C(OH)=N–, are ‘lactims’. Lactams are named in two ways:

(1) as heterocyclic pseudoketones;

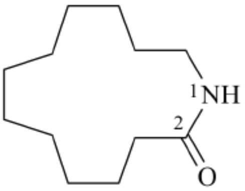
(2) by substituting ‘lactam’ for the ‘ic acid’ ending of a systematic ‘oic acid’ name for the parent acid without the amino substituent, and inserting a locant designating the position of the amino group between the ‘o’ and ‘lactam’. Lactims are named in the same way, using ‘lactim’ in place of ‘lactam’.

Method (1) generates preferred IUPAC names.

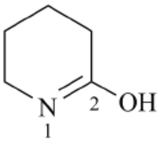
Examples:



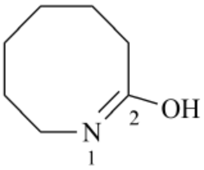
pyrrolidin-2-one (PIN)
butano-4-lactam



1-azacyclotridecan-2-one (PIN)
dodecano-12-lactam



3,4,5,6-tetrahydropyridin-2-ol (PIN)
pentano-5-lactim



3,4,5,6,7,8-hexahydroazocin-2-ol (PIN)
1,2-didehydroazocan-2-ol
heptano-7-lactim

P-66.1.5.2 Sultams, sultims, and intramolecular amides of sulfinic acids.

P-66.1.5.2.1 Intramolecular amides of amino sulfonic acids are called ‘sultams’ and may be named in three ways

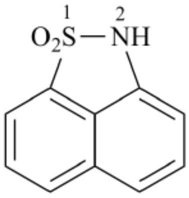
(1) as heterocyclic heterones;

(2) by citing the term ‘sultam’ denoting the cyclic –NH-SO_2– group after the name of the appropriate parent hydride preceded by a pair of locants describing the points of attachment of the sulfonyl group and the nitrogen atom, respectively; the locant of the sulfonyl group is cited first, and, if there is a choice, is the lower locant. Multiplying prefixes and pairs of locants separated by a colon are used to indicate two or more sultam rings;

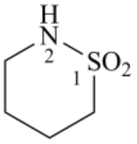
(3) as heterocycles and, according to functional class nomenclature, using the class term ‘oxide’.

Method (1) leads to preferred IUPAC names.

Examples:



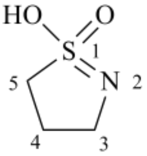
(1) 1λ^6^-naphtho[1,8-*cd*][1,2]thiazole-1,1(2*H*)-dione (PIN)
(3) 2*H*-naphtho[1,8-*cd*][1,2]thiazole 1,1-dioxide
(2) naphthalene-1,8-sultam



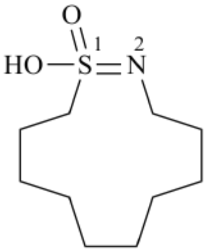
(1) 1λ^6^,2-thiazinane-1,1-dione (PIN)
(3) 1,2-thiazinane 1,1-dioxide
(2) butane-1,4-sultam

P-66.1.5.2.2 Sultims are tautomers of sultams and are named as described in P-66.1.5.2.1 for sultams, using the term ‘sultim’ in place of ‘sultam’.

Examples:



(1) 1-hydroxy-4,5-dihydro-3*H*-1λ^6^,2-thiazol-1-one (PIN)
(3) 1-hydroxy-4,5-dihydro-3*H*-1λ^4^,2-thiazole 1-oxide
(2) propane-1,3-sultim

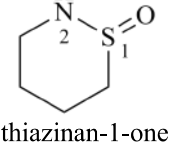


(1) 1-hydroxy-1λ^6^-thia-2-azacyclododec-1-en-1-one (PIN)
(3) 1-hydroxy-1λ^4^-thia-2-azacyclododec-1-ene 1-oxide
(2) decane-1,10-sultim

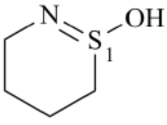
P-66.1.5.2.3 Intramolecular amides of amino sulfinic acids.

Cyclic amides of amino sulfinic acids and their tautomers are named as heterocyclic compounds.

Examples:



1λ^4^,2-thiazinan-1-one (PIN)
1,2-thiazinane 1-oxide



3,4,5,6-tetrahydro-1λ^4^,2-thiazin-1-ol (PIN)

P-66.1.6 Amides derived from carbonic, cyanic, and the di- and polycarbonic acids

P-66.1.6.1 Amides derived from carbonic acid and related compounds

P-66.1.6.1.1 Urea and its substitutive derivatives
P-66.1.6.1.2 Isourea and its derivatives
P-66.1.6.1.3 Chalcogen analogues of urea and isourea
P-66.1.6.1.4 Condensed ureas

P-66.1.6.1.1 Urea and its substitutive derivatives

P-66.1.6.1.1.1 The compound $H_2N\text{-}CO\text{-}NH_2$ has the retained name 'urea', which is the preferred IUPAC name, with locants *N* and *N*′, as shown above the structure below. The systematic name is 'carbonic diamide'. The locants 1, 2, and 3 have been used in the past and may be used in general nomenclature.

$$H_2\underset{1}{\overset{N}{N}}\text{-}\underset{2}{C}O\text{-}\underset{3}{\overset{N'}{N}}H_2$$

urea (PIN)

$$H_2\overset{N}{N}\text{-}CO\text{-}\overset{N'}{N}H_2$$

carbonic diamide

Numerical locants for urea are no longer used in the IUPAC preferred name.

P-66.1.6.1.1.2 Derivatives of urea formed by substitution on the nitrogen atom(s) are named as substitution products in accordance with the seniority order of urea that is ranked as an amide of carbonic acid. Amides of cyanic and the di- and polycarbonic acids follow the same seniority as the corresponding acid (see P-42.2).

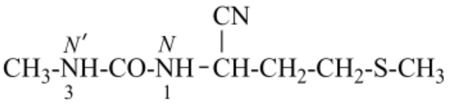
Examples:

$$CH_3\text{-}\underset{1}{\overset{N}{N}}H\text{-}\underset{2}{C}O\text{-}\underset{3}{\overset{N'}{N}}H\text{-}CH_3$$

N,*N*′-dimethylurea (PIN)
N,*N*′-dimethylcarbonic diamide

$$H_2N\text{-}CO\text{-}\overset{N}{N}{=}C(CH_3)_2$$

N-(propan-2-ylidene)urea (PIN)
isopropylideneurea
N-(propan-2-ylidene)carbonic diamide



$$CH_3\text{-}\underset{3}{\overset{N'}{N}}H\text{-}CO\text{-}\underset{1}{\overset{N}{N}}H\text{-}\overset{\overset{CN}{|}}{C}H\text{-}CH_2\text{-}CH_2\text{-}S\text{-}CH_3$$

N-[1-cyano-3-(methylsulfanyl)propyl]-*N*′-methylurea (PIN)
N-[1-cyano-3-(methylsulfanyl)propyl]-*N*′-methylcarbonic diamide

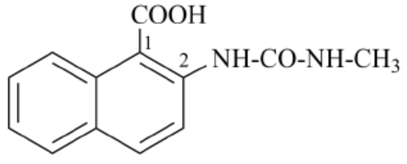
P-66.1.6.1.1.3 The prefixes for appropriate substituent groups derived from urea are formed systematically. The prefixes 'ureido' and 'ureylene' are not recommended.

The prefixes 'ureido' and 'ureylene' are no longer acceptable in IUPAC nomenclature. The prefixes 'carbamoylamino' and 'carbonylbis(azanediyl)', respectively are recommended for preferred IUPAC names.

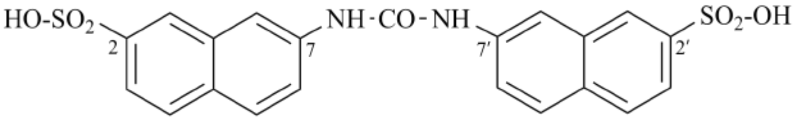
$H_2N\text{-}CO\text{-}NH–$
carbamoylamino (preferred prefix)
(aminocarbonyl)amino
(not ureido)

$–HN\text{-}CO\text{-}NH–$
carbonylbis(azanediyl)
(preferred prefix; for use in multiplicative nomenclature)
(not ureylene)

Examples:



2-[(methylcarbamoyl)amino]naphthalene-1-carboxylic acid (PIN)
2-{[(methylamino)carbonyl]amino}-1-naphthoic acid
[not 2-(3-methylureido)naphthalene-1-carboxylic acid]



7,7′-[carbonylbis(azanediyl)]di(naphthalene-2-sulfonic acid) (PIN)
[not 7,7′-ureylenedi(naphthalene-2-sulfonic acid)]

$C_6H_5\text{-CO-}\overset{N}{\text{N}}\text{H-CO-NH}_2$
N-carbamoylbenzamide (PIN)
N-(aminocarbonyl)benzamide

$C_6H_5\text{-SO}_2\text{-}\overset{N}{\text{N}}\text{H-CO-NH}_2$
N-carbamoylbenzenesulfonamide (PIN)
N-(aminocarbonyl)benzenesulfonamide

$H_2\text{N-CO-}\overset{N}{\text{N}}\text{H-}\overset{1}{\text{C}}\text{O-}\overset{2}{\text{C}}\text{H}_2\text{-C}_6\text{H}_5$
N-carbamoyl-2-phenylacetamide (PIN)
N-(aminocarbonyl)-2-phenylacetamide

P-66.1.6.1.1.4 Carboxylic acid derivatives of urea

Two carboxylic acids are related to urea; have been known as ‘allophanic acid’ for H_2N-CO-NH-COOH and ‘hydantoic acid’ for H_2N-CO-NH-CH_2-COOH. These names are no longer recommended. Preferred IUPAC names for these two acids and their derivatives are formed systematically.

Examples:

H_2N-CO-NH-COOH
carbamoylcarbamic acid (PIN)
(aminocarbonyl)carbamic acid

H_2N-CO-NH-CO–
carbamoylcarbamoyl (preferred prefix)
[(aminocarbonyl)amino]carbonyl

H_2N-CO-NH-CH_2-COOH
N-carbamoylglycine
(carbamoylamino)acetic acid

P-66.1.6.1.1.5 Seniority order of urea among amides

Amides are ranked in the same way as the corresponding acids (see P-42). Thus, in substitutive nomenclature, amides from carboxylic acids, including formamide, are senior to urea.

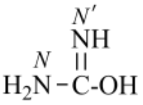
Examples:

$H_2\text{N-CO-NH-CH}_2\text{-CH}_2\text{-}\overset{N}{\text{N}}\text{H-CO-CH}_3$
N-[2-(carbamoylamino)ethyl]acetamide (PIN)
N-{2-[(aminocarbonyl)amino]ethyl}acetamide

H_2N-CO-NH-CH_2-CH_2-CH_2-NH-CHO
N-[3-(carbamoylamino)propyl]formamide (PIN)
[not *N*-(3-formamidopropyl)urea
nor *N*-[3-(formylamino)propyl]urea;
formamide is preferred to urea, see P-41]

P-66.1.6.1.2 Isourea and its derivatives

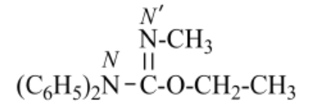
P-66.1.6.1.2.1 The imidic acid tautomer of urea, H_2N-C(OH)=NH, is named ‘carbamimidic acid’, a shortened form of the systematic functional replacement name ‘carbonamidimidic acid’. The name ‘isourea’ is no longer recommended, but is retained as a class name. In preferred IUPAC names, derivatives of carbamimidic acid are named using the locants *N* and *N*′. Since the name isourea is no longer recommended, even for general nomenclature, no numerical locants used in previous recommendations are needed. When the position of the double bond is unknown, only the locant *N* is used.



$$\mathrm{H_2\overset{\mathit{N}}{N}-\overset{\overset{\overset{\mathit{N'}}{NH}}{\|}}{C}-OH}$$

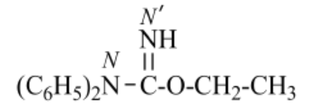
carbamimidic acid (PIN)
(not isourea)

Examples:



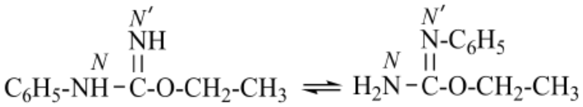
$$\mathrm{(C_6H_5)_2\overset{\mathit{N}}{N}-\overset{\overset{\overset{\mathit{N'}}{N-CH_3}}{\|}}{C}-O-CH_2-CH_3}$$

ethyl *N*′-methyl-*N*,*N*-diphenylcarbamimidate(PIN)
(not *O*-ethyl-*N*′-methyl-*N*,*N*-diphenylisourea)



$$\mathrm{(C_6H_5)_2\overset{\mathit{N}}{N}-\overset{\overset{\overset{\mathit{N'}}{NH}}{\|}}{C}-O-CH_2-CH_3}$$

ethyl *N*,*N*-diphenylcarbamimidate (PIN)
(not *O*-ethyl-*N*,*N*-diphenylisourea)



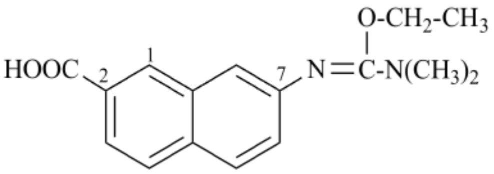
$$\mathrm{C_6H_5-\overset{\mathit{N}}{N}H-\overset{\overset{\overset{\mathit{N'}}{NH}}{\|}}{C}-O-CH_2-CH_3} \rightleftharpoons \mathrm{H_2\overset{\mathit{N}}{N}-\overset{\overset{\overset{\mathit{N'}}{N-C_6H_5}}{\|}}{C}-O-CH_2-CH_3}$$

ethyl *N*-phenylcarbamimidate (PIN)
(not *O*-ethyl-*N*-phenylisourea)

P-66.1.6.1.2.2 The groups HN=C(OH)-NH– and H_2N-C(OH)=N– derived from isourea are named respectively ‘(*C*-hydroxycarbonimidoyl)amino’ (preferred prefix) or [hydroxy(imino)methyl]amino-, and ‘[amino(hydroxy)methylidene]amino’ (preferred prefix). The italic letter locant ‘C’ is used in the preferred prefix to prevent possible ambiguity with *N*-substitution and parentheses are used around ‘hydroxy’ to emphasize that ‘amino’ is not substituted by ‘hydroxy’.

The prefixes 1-isoureido and 3-isoureido are no longer recommended.

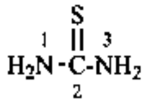
Example:



7-{[(dimethylamino)ethoxymethylidene]amino}naphthalene-2-carboxylic acid (PIN)
[not 7-(2-ethyl-1,1-dimethyl-3-isoureido)naphthalene-2-carboxylic acid]

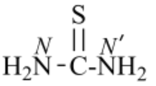
P-66.1.6.1.3 Chalcogen analogues of urea and isourea

P-66.1.6.1.3.1 Chalcogen analogues of urea are named by functional replacement nomenclature using the prefixes ‘thio’, ‘seleno’, and ‘telluro’. Preferred IUPAC names use the letter locants *N*, and *N*′. Numerical locants may be used for thiourea in general nomenclature.



$$\mathrm{H_2\overset{1}{N}-\underset{2}{\overset{\overset{S}{\|}}{C}}-\overset{3}{N}H_2}$$

caronothioic diamide

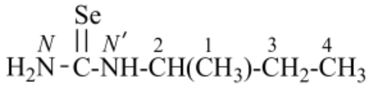


$$\mathrm{H_2\overset{\mathit{N}}{N}-\overset{\overset{S}{\|}}{C}-\overset{\mathit{N'}}{N}H_2}$$

thiourea (PIN)

Numerical locants are no longer used for thiourea in the IUPAC preferred name.

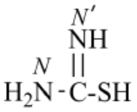
Example:



$$\mathrm{H_2\overset{\mathit{N}}{N}-\overset{\overset{Se}{\|}}{C}-\overset{\mathit{N'}}{N}H-\overset{2}{C}H(\overset{1}{C}H_3)-\overset{3}{C}H_2-\overset{4}{C}H_3}$$

N-(butan-2-yl)selenourea (PIN)
N-(1-methylpropyl)selenourea
N-(butan-2-yl)carbonoselenoic diamide

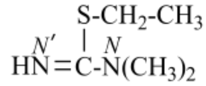
P-66.1.6.1.3.2 Chalcogen analogues of isourea are named by functional replacement nomenclature using the appropriate chalcogen infixes, for example, carbamimidothioic acid, not isothiourea. The italic locants *N*, and *N′* are used for preferred IUPAC names. When the position of the double bond is not known, locants *S* or *Se* or *Te* and *N* are used to assign substituents to appropriate atoms.



$$\mathrm{H_2}\overset{N}{\mathrm{N}}\text{-}\overset{\overset{N'}{\mathrm{NH}}}{\overset{\|}{\mathrm{C}}}\text{-SH}$$

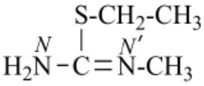
carbamimidothioic acid (PIN)
(not isothiourea)

Examples:



$$\overset{N'}{\mathrm{HN}}{=}\overset{\overset{\text{S-CH}_2\text{-CH}_3}{|}}{\mathrm{C}}\text{-}\overset{N}{\mathrm{N}}(\mathrm{CH_3})_2$$

ethyl *N*,*N*-dimethylcarbamimidothioate (PIN)
(not *S*-ethyl-*N*,*N*-dimethylisothiourea)



$$\mathrm{H_2}\overset{N}{\mathrm{N}}\text{-}\overset{\overset{\text{S-CH}_2\text{-CH}_3}{|}}{\mathrm{C}}{=}\overset{N'}{\mathrm{N}}\text{-CH}_3$$

ethyl *N′*-methylcarbamimidothioate (PIN)
(not *S*-ethyl-*N′*-methylisothiourea)

For the example just above, when the position of the double bond is not known the names would be:

ethyl *N*-methylcarbamimidothioate (PIN)
(not *S*-ethyl-*N*-methylisothiourea)

P-66.1.6.1.3.3 Prefixes for substituents derived from chalcogen analogues of urea and isourea are as follows:

$\mathrm{H_2N}$-CS-NH–	carbamothioylamino (preferred prefix) [amino(sulfanylidene)methyl]amino-
HN=C(SH)-NH–	(*C*-sulfanylcarbonimidoyl)amino (preferred prefix) [imino(sulfanyl)methyl]amino-
$\mathrm{H_2N}$-C(SH)=N–	[amino(sulfanyl)methylidene]amino (preferred prefix)

Example:

$$\mathrm{H_2N\text{-}CS\text{-}NH\text{-}}\overset{3}{\mathrm{C}}\mathrm{H_2\text{-}}\overset{2}{\mathrm{C}}\mathrm{H_2\text{-}}\overset{1}{\mathrm{C}}\mathrm{OOH}$$

3-(carbamothioylamino)propanoic acid (PIN)
3-{[amino(sulfanylidene)methyl]amino}propanoic acid

P-66.1.6.1.4 Condensed ureas

Condensed ureas, $\mathrm{H_2N\text{-}[CO\text{-}NH]}_n\text{-H}$, where n = 2, 3, or 4, are named systematically as diamides of imidodicarbonic acid, diimidotricarbonic acid, and triimidotetracarbonic acid, etc., functional replacement names derived from the corresponding di- or polycarbonic acids. The names biuret, triuret, etc., are no longer recommended as preferred IUPAC names. Chalcogen analogues are described by functional replacement prefixes alphabetized along with 'imido' in front of the corresponding di- or polycarbonic acid. Locants, as shown above the structures, below, are used to indicate the positions of substituents and functional replacement prefixes, where needed. Preferred IUPAC names use these locants which are also prescribed for the amides of imidopolycarbonic acids (see P-66.4.1.2.2). The full numerical numbering system used previously and shown below the structures may be used in general nomenclature.

$$\overset{N^1}{\underset{1}{\mathrm{H_2N}}}\text{-}\overset{1}{\underset{2}{\mathrm{CO}}}\text{-}\overset{2}{\underset{3}{\mathrm{NH}}}\text{-}\overset{3}{\underset{4}{\mathrm{CO}}}\text{-}\overset{N^3}{\underset{5}{\mathrm{NH_2}}}$$

2-imidodicarbonic diamide (PIN)
biuret

$$\overset{N^1}{\underset{1}{\mathrm{H_2N}}}\text{-}\overset{1}{\underset{2}{\mathrm{CO}}}\text{-}\overset{2}{\underset{3}{\mathrm{NH}}}\text{-}\overset{3}{\underset{4}{\mathrm{CO}}}\text{-}\overset{4}{\underset{5}{\mathrm{NH}}}\text{-}\overset{5}{\underset{6}{\mathrm{CO}}}\text{-}\overset{N^5}{\underset{7}{\mathrm{NH_2}}}$$

2,4-diimidotricarbonic diamide (PIN)
triuret

Numerical locants for condensed ureas are no longer used in IUPAC preferred names.

Examples:

$$\mathrm{CH_3\text{-}\underset{1}{\overset{\mathit{N}^1}{N}}H\text{-}\overset{1}{C}O\text{-}\overset{2}{N}H\text{-}\overset{3}{C}O\text{-}\overset{\mathit{N}^3}{N}H_2}$$

*N*¹-methyl-2-imidodicarbonic diamide (PIN)
1-methylbiuret

$$\mathrm{CH_3\text{-}\underset{1}{\overset{\mathit{N}^1}{N}}H\text{-}\underset{2}{\overset{1}{C}}S\text{-}\overset{2}{N}H\text{-}\overset{3}{C}O\text{-}\overset{\mathit{N}^3}{N}H_2}$$

*N*¹-methyl-2-imido-1-thiodicarbonic diamide (PIN)
1-methyl-2-thiobiuret

$$\mathrm{CH_3\text{-}\underset{1}{\overset{\mathit{N}^1}{N}}H\text{-}\overset{1}{C}O\text{-}\overset{2}{N}H\text{-}\underset{4}{\overset{3}{C}}S\text{-}\overset{4}{N}H\text{-}\overset{5}{C}O\text{-}\overset{\mathit{N}^5}{N}H_2}$$

*N*¹-methyl-2,4-diimido-3-thiotricarbonic diamide (PIN)
1-methyl-4-thiotriuret

For polyurets, where *n* = 5 and higher, skeletal replacement (‘a’) nomenclature leads to preferred IUPAC names.

Example:

$$\mathrm{H_2N\text{-}\overset{1}{C}O\text{-}\overset{2}{N}H\text{-}\overset{3}{C}O\text{-}\overset{4}{N}H\text{-}\overset{5}{C}O\text{-}\overset{6}{N}H\text{-}\overset{7}{C}O\text{-}\overset{8}{N}H\text{-}\overset{9}{C}O\text{-}NH_2}$$

3,5,7-trioxo-2,4,6,8-tetraazanonane-1,9-diamide (PIN)
pentauret

P-66.1.6.2 Amides derived from cyanic acid

The traditional name ‘cyanamide’ is retained for $\mathrm{NC\text{-}NH_2}$ and is the preferred IUPAC name. Substitution is allowed on the $\mathrm{–NH_2}$ group. The systematic functional replacement name is carbononitridic amide.

Examples:

$\mathrm{NC\text{-}NH\text{-}CH(CH_3)_2}$
(propan-2-yl)cyanamide (PIN)
(propan-2-yl)carbononitridic amide

$\mathrm{NC\text{-}N(CH_2\text{-}CH_3)_2}$
diethylcyanamide (PIN)
diethylcarbononitridic amide

P-66.1.6.3 Amides of di- and polycarbonic acids

Systematic names for amides of the polycarbonic acids are formed by adding the functional class name ‘amide’ to that of the corresponding acid, preceded by the numerical prefix ‘di’ to indicate the presence of two $\mathrm{–NH_2}$ groups. Chalcogen analogues are described by functional replacement prefixes. Numerical and letter locants are used to number the structures.

$$\mathrm{H_2\overset{\mathit{N}^1}{N}\text{-}\overset{1}{C}O\text{-}\overset{2}{O}\text{-}\overset{3}{C}O\text{-}\overset{\mathit{N}^3}{N}H_2}$$

dicarbonic diamide (PIN)

$$\mathrm{H_2\overset{\mathit{N}^1}{N}\text{-}\overset{1}{C}O\text{-}\overset{2}{O}\text{-}\overset{3}{C}O\text{-}\overset{4}{O}\text{-}\overset{5}{C}O\text{-}\overset{\mathit{N}^5}{N}H_2}$$

tricarbonic diamide (PIN)

Examples:

$$\mathrm{(CH_3)_2CH\text{-}\overset{\mathit{N}^1}{N}H\text{-}\overset{1}{C}O\text{-}\overset{2}{O}\text{-}\overset{3}{C}O\text{-}\overset{\mathit{N}^3}{N}H_2}$$

*N*¹-(propan-2-yl)dicarbonic diamide (PIN)
N-isopropyldicarbonic diamide

$$\mathrm{CH_3\text{-}\overset{\mathit{N}^1}{N}H\text{-}\overset{1}{C}O\text{-}\overset{2}{S}\text{-}\overset{3}{C}O\text{-}\overset{4}{O}\text{-}\overset{5}{C}O\text{-}\overset{\mathit{N}^5}{N}H_2}$$

*N*¹-methyl-2-thiotricarbonic diamide (PIN)

$$\mathrm{H_2\overset{\mathit{N}^1}{N}\text{-}\overset{1}{C}S\text{-}\overset{2}{S}\text{-}\overset{3}{C}S\text{-}\overset{\mathit{N}^3}{N}H_2}$$

1,2,3-trithiodicarbonic diamide (PIN)
(not ‘thiuram monosulfide’)

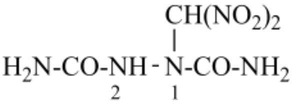
$$\overset{N^1}{H_2N}\text{-}\overset{1}{C}S\text{-}\overset{2}{S}\text{-}S\text{-}\overset{3}{C}S\text{-}\overset{N^3}{NH_2}$$

2-dithioperoxy-1,3-dithiodicarbonic diamide (PIN)
(not ‘thiuram disulfide’)

P-66.1.7 Polyfunctional amides

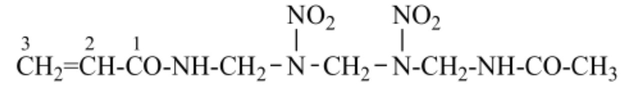
Amides follow acids, anhydrides, esters, and acid halides in the seniority order of compound classes expressed by suffixes (see P-41); within the amide class, amides rank in the same order as the corresponding acid. Seniority for numbering polyfunctional amides follows that described for acids, for which see P-65.1.2.3 and P-65.1.2.4.

Examples:



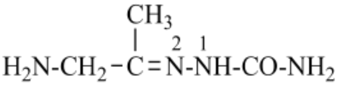
$$H_2N\text{-}CO\text{-}\underset{2}{NH}\text{-}\underset{1}{\overset{CH(NO_2)_2}{\overset{|}{N}}}\text{-}CO\text{-}NH_2$$

1-(dinitromethyl)hydrazine-1,2-dicarboxamide (PIN)



$$\overset{3}{C}H_2\text{=}\overset{2}{C}H\text{-}\overset{1}{C}O\text{-}NH\text{-}CH_2\text{-}\overset{NO_2}{\overset{|}{N}}\text{-}CH_2\text{-}\overset{NO_2}{\overset{|}{N}}\text{-}CH_2\text{-}NH\text{-}CO\text{-}CH_3$$

N-[({[(acetamidomethyl)nitramido]methyl}nitramido)methyl]prop-2-enamide (PIN)
N-{[{[(acetamidomethyl)(nitro)amino]methyl}(nitro)amino]methyl}prop-2-enamide
N-{[({[(acetylamino)methyl](nitro)amino}methyl)(nitro)amino]methyl}prop-2-enamide

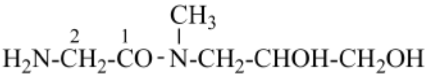


$$H_2N\text{-}CH_2\text{-}\overset{CH_3}{\overset{|}{C}}\text{=}\overset{2}{N}\text{-}\overset{1}{N}H\text{-}CO\text{-}NH_2$$

2-(1-aminopropan-2-ylidene)hydrazine-1-carboxamide (PIN)

$$HO\text{-}CH_2\text{-}CH_2\text{-}NH\text{-}\overset{4}{C}H_2\text{-}\overset{3}{C}H_2\text{-}\overset{2}{C}H_2\text{-}CO\text{-}NH\text{-}CH_2\text{-}CH_2\text{-}NH\text{-}CH_2\text{-}CH_2\text{-}OH$$

4-[(2-hydroxyethyl)amino]-*N*-{2-[(2-hydroxyethyl)amino]ethyl}butanamide (PIN)



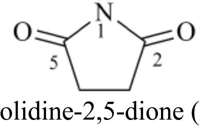
$$H_2N\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}O\text{-}\overset{CH_3}{\overset{|}{N}}\text{-}CH_2\text{-}CHOH\text{-}CH_2OH$$

2-amino-*N*-(2,3-dihydroxypropyl)-*N*-methylacetamide (PIN)

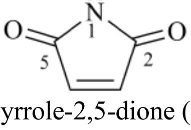
P-66.2 IMIDES

P-66.2.1 Imides are compounds containing the structural grouping –CO-NH-CO–. Acyclic imides are *N*-acyl derivatives of primary amides and are named as such (see P-66.1.2.1). Cyclic imides are preferably named as heterocyclic pseudoketones. They may also be named by replacing the suffixes ‘dioic acid’, or ‘dicarboxylic acid’ of the corresponding dibasic acid, or ‘ic acid’ in retained names of diacids, by ‘imide’ or ‘dicarboximide’.

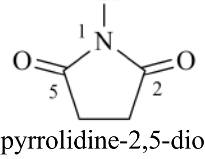
Examples:



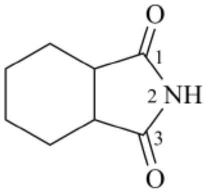
pyrrolidine-2,5-dione (PIN)
succinimide



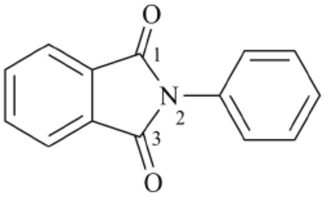
1*H*-pyrrole-2,5-dione (PIN)
pyrrole-2,5-dione



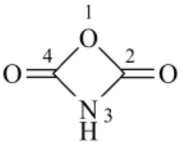
1-bromopyrrolidine-2,5-dione (PIN)
(not *N*-bromosuccinimide;
substitution is not allowed on succinimide)



hexahydro-1*H*-isoindole-1,3(2*H*)-dione (PIN)
hexahydro-2*H*-isoindole-1,3-dione
cyclohexane-1,2-dicarboximide

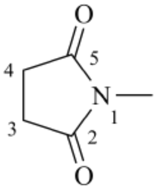


2-phenyl-1*H*-isoindole-1,3(2*H*)-dione (PIN)
2-phenyl-2*H*-isoindole-1,3-dione
N-phenylphthalimide



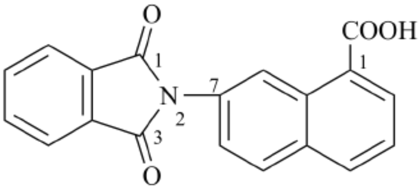
1,3-oxazetidine-2,4-dione (PIN)

P-66.2.2 Prefixes derived from imides by removal of the hydrogen atom attached to the imide nitrogen atom are named systematically as preferred prefixes. However, for general nomenclature they may be formed from the name of the corresponding imide by changing the ending 'imide' to 'imido'.



succinimido
2,5-dioxopyrrolidin-1-yl (preferred prefix)

Example:



7-phthalimido-1-naphthoic acid
7-(1,3-dioxo-1,3-dihydro-2*H*-isoindol-2-yl)naphthalene-1-carboxylic acid (PIN)

P-66.3 HYDRAZIDES

P-66.3.0 Definition
P-66.3.1 Systematic names
P-66.3.2 Substituent groups derived from hydrazides
P-66.3.3 Substituted hydrazides
P-66.3.4 Chalogen analogues of hydrazides
P-66.3.5 Hydrazides from carbonic, cyanic, and di- and polycarbonic acids
P-66.3.6 Semioxamazones

P-66.3.0 Definition

Hydrazides are compounds derived from the organic oxoacids denoted by a suffix, such as –COOH, $–SO_2$-OH, –SO-OH, etc., by replacing –OH groups with $–NH-NH_2$ groups.

P-66.3.1 Systematic names

Hydrazides of the type $R-CO-NH-NH_2$ are named in two ways:

(1) by substitutive nomenclature;

(2) by modification of retained names of carboxylic acids.

P-66.3.1.1 Substitutive nomenclature

Hydrazides are named substitutively by using the following suffixes (see Table 4.4). The method of naming hydrazides as acyl derivatives of hydrazine is no longer recommended.

$–(C)O\text{-}NH\text{-}NH_2$	hydrazide (preferred suffix)
$–CO\text{-}NH\text{-}NH_2$	carbohydrazide (preferred suffix)
$–SO_2\text{-}NH\text{-}NH_2$	sulfonohydrazide (and corresponding Se and Te analogues; preselected suffixes)
$–SO\text{-}NH\text{-}NH_2$	sulfinohydrazide (and corresponding Se and Te analogues; preselected suffixes)

> For naming acyclic hydrazides, the suffix 'hydrazide' is recommended in place of 'ohydrazide' in accordance with the general use of suffixes added to names of parent hydrides, for example pentanehydrazide for $CH_3\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}CO\text{-}NH\text{-}NH_2$, not pentanohydrazide.

The suffix 'hydrazide' is used to name acyclic compounds. The suffix 'carbohydrazide' is used to denote the $–CO\text{-}NH\text{-}NH_2$ characteristic group attached to cyclic compounds and in chains having more than two $–CO\text{-}NH\text{-}NH_2$ characteristic groups, or when the group is attached to a heteroatom of a heterocycle or parent compound. Multiplicative nomenclature may be used when the symmetry conditions for its use are met.

Nitrogen atoms in hydrazides are identified by the locants *N* and *N′* as $–CO\text{-}\overset{N}{N}H\text{-}\overset{N'}{N}H_2$, even though hydrazine itself, is numbered using the numerical locants 1 and 2, $H_2\overset{1}{N}\text{-}\overset{2}{N}H_2$. When two hydrazide suffixes are attached to an acyclic alkane, the suffix in position 1 is labeled N^1, N'^1, a second suffix in position 'x', N^x, N'^x (see P-16.9).

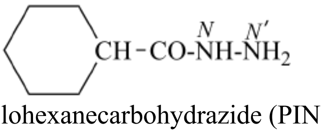
Examples:

$$\overset{5}{C}H_3\text{-}\overset{4}{C}H_2\text{-}\overset{3}{C}H_2\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}O\text{-}\overset{N}{N}H\text{-}\overset{N'}{N}H_2$$

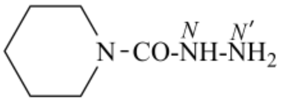
pentanehydrazide (PIN)
(not pentanoylhydrazine)

$$H_2\overset{N'^4}{N}\text{-}\overset{N^4}{N}H\text{-}\overset{4}{C}O\text{-}\overset{3}{C}H_2\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}O\text{-}\overset{N^1}{N}H\text{-}\overset{N'^1}{N}H_2$$

butanedihydrazide (PIN)
succinohydrazide (see P-66.3.1.2)
[not (ethane-1,2-diyldicarbonyl)dihydrazine]
[not succinyldihydrazine]



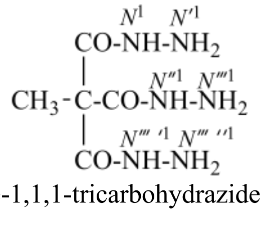
cyclohexanecarbohydrazide (PIN)
[not (cyclohexanecarbonyl)hydrazine]



piperidine-1-carbohydrazide (PIN)
[not (piperidine-1-carbonyl)hydrazine]

$$CH_3\text{-}SO_2\text{-}\overset{N}{N}H\text{-}\overset{N'}{N}H_2$$

methanesulfonohydrazide (PIN)
[not (methanesulfonyl)hydrazine]



$$\begin{array}{l} \quad\;\; CO\text{-}\overset{N^1}{N}H\text{-}\overset{N'^1}{N}H_2 \\ \quad\;\; | \\ CH_3\text{-}C\text{-}CO\text{-}\overset{N''^1}{N}H\text{-}\overset{N'''^1}{N}H_2 \\ \quad\;\; | \\ \quad\;\; CO\text{-}\overset{N'''\,'^1}{N}H\text{-}\overset{N'''\,''^1}{N}H_2 \end{array}$$

ethane-1,1,1-tricarbohydrazide (PIN)

P-66.3.1.2 Names formed by modifying retained names of carboxylic acids

Names of hydrazides are formed by changing the 'ic acid' or '-oic acid' ending of the retained names of carboxylic acids into 'ohydrazide' (for nitrogen locants, see P-66.3.3).

P-66.3.1.2.1 Only the following five names are preferred IUPAC names and can be substituted in the same way as corresponding amides (see P-66.1.1.1.2). Systematic substitutive names are used to generate acids modified by functional replacement.

$$\mathrm{NC\text{-}\overset{\mathit{N}}{N}H\text{-}\overset{\mathit{N'}}{N}H_2}$$

cyanohydrazide (PIN)
hydrazinecarbonitrile (see P-66.5.1.1.3)

$$\mathrm{HCO\text{-}\overset{\mathit{N}}{N}H\text{-}\overset{\mathit{N'}}{N}H_2}$$

formohydrazide (PIN)
(not hydrazinecarbaldehyde; see P-66.6.1.3)

$$\mathrm{CH_3\text{-}CO\text{-}\overset{\mathit{N}}{N}H\text{-}\overset{\mathit{N'}}{N}H_2}$$

acetohydrazide (PIN)

$$\mathrm{C_6H_5\text{-}CO\text{-}\overset{\mathit{N}}{N}H\text{-}\overset{\mathit{N'}}{N}H_2}$$

benzohydrazide (PIN)

$$\mathrm{H_2\overset{\mathit{N'^1}}{N}\text{-}\overset{\mathit{N^1}}{N}H\text{-}\overset{1}{C}O\text{-}\overset{2}{C}O\text{-}\overset{\mathit{N^2}}{N}H\text{-}\overset{\mathit{N'^2}}{N}H_2}$$

oxalohydrazide (PIN)

Hydrazides of the -imidic and -hydrazonic analogues of these acids are named systematically.

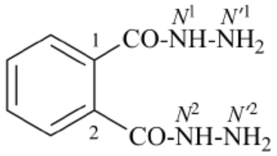
Example:

$$\mathrm{CH_3\text{-}C(=NH)\text{-}NH\text{-}NH_2}$$

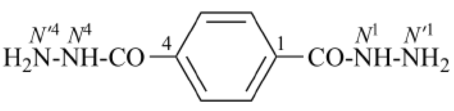
ethanimidohydrazide (PIN)
(not acetimidohydrazide)

P-66.3.1.2.2 For general nomenclature, only the names furohydrazide, phthalohydrazide, isophthalohydrazide, and terephthalohydrazide are retained with limited substitution allowed (see P-65.1.1.2); the corresponding systematic names are preferred IUPAC names (see P-66.3.1.1). When two or more 'carbohydrazide' suffixes are present, the nitrogen locants are *N* and *N'* with appropriate superscript numerical locants denoting the locants of the parent structure.

Examples:



benzene-1,2-dicarbohydrazide (PIN)
phthalohydrazide



benzene-1,4-dicarbohydrazide (PIN)
terephthalohydrazide

P-66.3.1.2.3 For retained names for carboxylic acids used only in general nomenclature (see P-65.1.1.2.1), hydrazide formation is governed by the above rule, P-66.3.1.2.1; but substitution is not allowed, including substitution on the nitrogen atom(s) of the hydrazide characteristic group. Systematic names are preferred IUPAC names (see P-66.3.1.1).

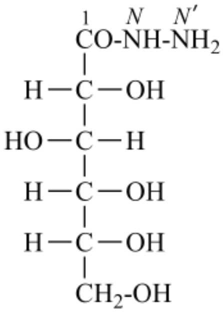
Example:

$$\mathrm{CH_3\text{-}CH_2\text{-}CH_2\text{-}CO\text{-}\overset{\mathit{N}}{N}H\text{-}\overset{\mathit{N'}}{N}H_2}$$

butanehydrazide (PIN)
butyrohydrazide
(substitution not allowed)

P-66.3.1.2.4 Hydrazides derived from carbohydrate acids and α-amino acids are discussed in P-102.5.6.6.2.1 and P-103.2.7, respectively.

Examples:



D-gluconohydrazide

$H_2N\text{-}\overset{2}{C}H_2\text{-}CO\text{-}\overset{N}{N}H\text{-}\overset{N'}{N}H_2$

2-aminoacetohydrazide
glycinohydrazide

P-66.3.2 Substituent groups derived from hydrazides

Substituent groups corresponding to hydrazides are of two types: –CO-NH-NH₂, –SO₂-NH-NH₂, etc.; and –NH-NH-CO-R, –NH-NH-SO₂-R, etc.

P-66.3.2.1 Substituent groups of the type –CO-NH-NH₂, –SO₂-NH-NH₂, etc., may be named in three ways except when the –CO-NH-NH₂ group is at the end of a carbon chain:

(1) as an acyl group derived from the corresponding acid, which gives the preferred prefix; or

(2) as the appropriate carbonohydrazidoyl acyl prefix; or

(3) by concatenation using the prefix hydrazinyl with carbonyl.

Examples:

$H_2\overset{2}{N}\text{-}\overset{1}{N}H\text{-}COOH$

hydrazinecarboxylic acid (PIN)
carbonohydrazidic acid

$H_2\overset{2}{N}\text{-}\overset{1}{N}H\text{-}CO\text{–}$

(1) hydrazinecarbonyl (preferred prefix)
(2) carbonohydrazidoyl (see P-65.2.1.4)
(3) hydrazinylcarbonyl

$H_2\overset{2}{N}\text{-}\overset{1}{N}H\text{-}SO_2\text{-}OH$

hydrazinesulfonic acid (preselected name)

$H_2\overset{2}{N}\text{-}\overset{1}{N}H\text{-}SO_2\text{–}$

(1) hydrazinesulfonyl (preselecteded prefix, see P-65.3.2.2.2)
(3) hydrazinylsulfonyl

$H_2\overset{2}{N}\text{-}\overset{1}{N}H\text{-}SO\text{-}OH$

hydrazinesulfinic acid (preselected name)

$H_2\overset{2}{N}\text{-}\overset{1}{N}H\text{-}SO\text{–}$

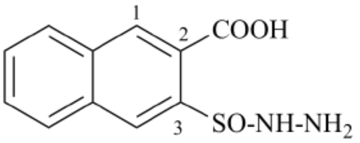
(1) hydrazinesulfinyl (preselecteded prefix: see P-65.3.2.2.2)
(3) hydrazinylsulfinyl

Method (1) leads to preferred prefixes.

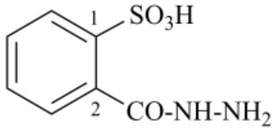
Examples:

$H_2\overset{2}{N}\text{-}\overset{1}{N}H\text{-}SO_2\text{-}CH_2\text{-}COOH$

(hydrazinesulfonyl)acetic acid (PIN)
(hydrazinylsulfonyl)acetic acid



3-(hydrazinesulfinyl)naphthalene-2-carboxylic acid (PIN)
3-(hydrazinylsulfinyl)naphthalene-2-carboxylic acid



2-(hydrazinecarbonyl)benzene-1-sulfonic acid (PIN)
2-carbonohydrazidoylbenzene-1-sulfonic acid

P-66.3.2.2 When the –CO-NHNH$_2$ group is at the end of a chain the use of the prefixes ‘hydrazinyl’ and ‘oxo’ generates preferred IUPAC names.

Example:

$$\mathrm{H_2N\text{-}NH\text{-}\overset{3}{C}O\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}OOH}$$

3-hydrazinyl-3-oxopropanoic acid (PIN)
(hydrazinecarbonyl)acetic acid
carbonohydrazidoylacetic acid

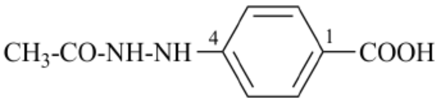
P-66.3.2.3 When a group having priority for citation as a principal characteristic group is present, a hydrazide group of the type R-CO-NH-NH– or R-SO$_2$-NH-NH– (or the analogous selenium or tellurium group) is named:

(1) by expressing the corresponding hydrazide as a prefix by replacing the final letter ‘e’ in the name of the hydrazide by the letter ‘o’, for example, ‘acetohydrazido’, ‘propanehydrazido’, and ‘benzohydrazido’; the locant *N* designates the nitrogen atom adjacent to the –CO– group.

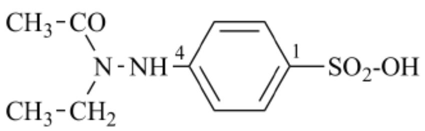
(2) as an acylhydrazinyl substituent group; the hydrazinyl group is numbered by using numerical locants ‘1’ and ‘2’, the locant ‘1’ being the nitrogen atom adjacent to the free valence.

Method (1) generates preferred IUPAC names.

Examples:



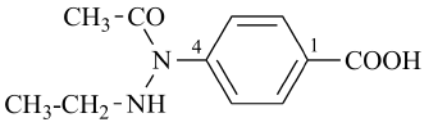
(1) 4-acetohydrazidobenzoic acid (PIN)
(2) 4-(2-acetylhydrazin-1-yl)benzoic acid



(1) 4-(*N*-ethylacetohydrazido)benzene-1-sulfonic acid (PIN)
(2) 4-(2-acetyl-2-ethylhydrazin-1-yl)benzene-1-sulfonic acid

The groups R-CO-N(NH$_2$)–, R-SO$_2$N(NH$_2$)–, etc. are named as substituted derivatives of the group ‘hydrazinyl,’ with numerical locants. This method leads to preferred prefixes.

Example:



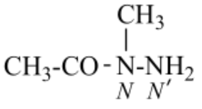
4-(1-acetyl-2-ethylhydrazin-1-yl)benzoic acid (PIN)

P-66.3.3 Substituted hydrazides

P-66.3.3.1 Alkyl, aryl, cycloalkyl, etc. substituents on the nitrogen atoms of hydrazides are described by the appropriate prefix names and the locants ‘*N*’ for –NH– and ‘*N*′’ for –NH$_2$, as illustrated below. The locants ‘1′’and ‘2′’ have been used in the past for naming hydrazides as derivatives of hydrazine; these locants are no longer recommended. Preferred IUPAC names are hydrazide names and use the locants ‘*N*’ and ‘*N*′’

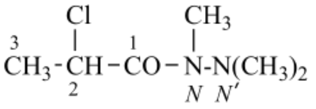
$$\mathrm{CH_3\text{-}CH_2\text{-}CO\text{-}\overset{\mathit{N}}{N}H\text{-}\overset{\mathit{N'}}{N}H_2}$$

Examples:



$$CH_3\text{-}CO\text{-}\underset{N}{\overset{\overset{CH_3}{|}}{N}}\text{-}\underset{N'}{NH_2}$$

N-methylacetohydrazide (PIN)
(not 1-acetyl-1-methylhydrazine)

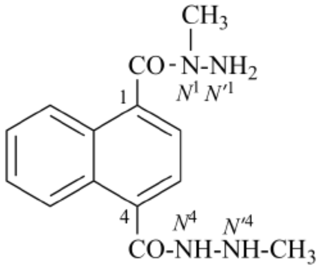


$$\overset{3}{CH_3}\text{-}\underset{2}{\overset{\overset{Cl}{|}}{CH}}\text{-}\overset{1}{CO}\text{-}\underset{N}{\overset{\overset{CH_3}{|}}{N}}\text{-}\underset{N'}{N}(CH_3)_2$$

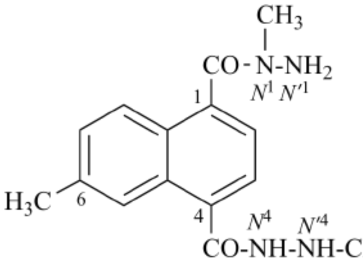
2-chloro-*N*,*N'*,*N'*-trimethylpropanehydrazide (PIN)
[not 1-(2-chloropropanoyl)-1,2,2-trimethylhydrazine]

P-66.3.3.2 When two hydrazide groups are present, each is identified by the locants *N* and *N'*. To distinguish the four nitrogen atoms, the numerical locant of the position on the parent structure at which the nitrogen atoms are attached is cited as a superscript to the letter locant *N* or *N'* for example, N^1, N'^1, etc. (see also P-62.2.4.1.2).

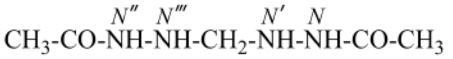
Examples:



N^1,N'^4-dimethylnaphthalene-1,4-dicarbohydrazide (PIN)
(numbering is based on the lower set of locants:
since N^1 is lower than N'^1; the set N^1,N'^4 is lower than N'^1,N^4)



N^1,N'^4,6-trimethylnaphthalene-1,4-dicarbohydrazide (PIN)
(the numbering is based on the lowest set of locants for the three substituent groups,
and 'N^1,N'^4,6' is lower than 'N'^1,N^4,7')

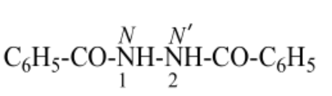


$$CH_3\text{-}CO\text{-}\overset{N''}{NH}\text{-}\overset{N'''}{NH}\text{-}CH_2\text{-}\overset{N'}{NH}\text{-}\overset{N}{NH}\text{-}CO\text{-}CH_3$$

N',*N'''*-methylenediacetohydrazide (PIN, a multiplicative name)

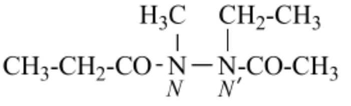
P-66.3.3.3 Acyl, diacyl, and triacyl derivatives of hydrazides are named by substituting the senior hydrazide by the appropriate acyl groups (the senior hydrazide is the one derived from the senior acid). Names based on substitution of the parent hydride 'hydrazine' are no longer recommended even in general nomenclature. Hydrazine, a retained name, is preferred to diazane for preferred IUPAC names.

Examples:



$$C_6H_5\text{-}CO\text{-}\underset{1}{\overset{N}{NH}}\text{-}\underset{2}{\overset{N'}{NH}}\text{-}CO\text{-}C_6H_5$$

N'-benzoylbenzohydrazide (PIN)
(not 1,2-dibenzoylhydrazine)



$$CH_3\text{-}CH_2\text{-}CO\text{-}\underset{N}{\overset{\overset{H_3C}{|}}{N}}-\underset{N'}{\overset{\overset{CH_2\text{-}CH_3}{|}}{N}}\text{-}CO\text{-}CH_3$$

N'-acetyl-*N'*-ethyl-*N*-methylpropanehydrazide (PIN)
(not 1-acetyl-1-ethyl-2-methyl-2-propanoylhydrazine)

P-66.3.4 Chalcogen analogues of hydrazides

Chalcogen analogues of hydrazides are named substitutively using suffixes formed by functional replacement, i.e., 'thiohydrazide', 'carbothiohydrazide', 'sulfonothiohydrazide', etc., as described in P-33.2.2 and Table 4.4.

The following methods are no longer recommended:

(a) substitution of hydrazine with appropriately modified acyl groups;

(b) modification of retained names by the prefixes ‘thio’, ‘seleno’, ‘telluro’.

Examples:

$$CH_3\text{-}CH_2\text{-}CS\text{-}\overset{N}{N}H\text{-}\overset{N'}{N}H_2$$

propanethiohydrazide (PIN)
[not (propanethioyl)hydrazine;
nor (thiopropionyl)hydrazine]

$$C_6H_5\text{-}CS\text{-}\overset{N}{N}H\text{-}\overset{N'}{N}H_2$$

benzenecarbothiohydrazide (PIN)
[not (benzenecarbothioyl)hydrazine;
nor (thiobenzoyl)hydrazine]

$$H_2\overset{N'}{N}\text{-}\overset{N}{N}H\text{-}\overset{1}{C}O\text{-}\overset{2}{C}S\text{-}NH\text{-}NH_2$$

2-hydrazinyl-2-sulfanylideneacetohydrazide (PIN)
(not thiooxalic dihydrazide)

P-66.3.5 Hydrazides from carbonic, cyanic, and di- and polycarbonic acids

P-66.3.5.1 Preferred IUPAC names for hydrazides derived from carbonic and cyanic acids are chosen according to the seniority order of classes.

Examples:

$$H_2\overset{2}{N}\text{-}\overset{1}{N}H\text{-}CN$$

cyanohydrazide (PIN)
[cyanic acid is a retained name (see P-65.2.2)]
carbononitridic hydrazide
hydrazinecarbonitrile

$$H_2\overset{2}{N}\text{-}\overset{1}{N}H\text{-}COOH$$

hydrazinecarboxylic acid (PIN)
carbonohydrazidic acid

$$H_2\overset{2}{N}\text{-}\overset{1}{N}H\text{-}CO\text{-}\overset{N}{N}H\text{-}\overset{N'}{N}H_2$$

hydrazinecarbohydrazide (PIN)
carbonic dihydrazide

P-66.3.5.2 Names of hydrazides derived from the di- and polycarbonic acids are formed by adding the functional class name ‘hydrazide’ to that of the corresponding acid, preceded by the numerical prefix ‘di’ to express multiplicity of hydrazide groups, when necessary. Chalcogen and other replacement analogues are described by the appropriate functional replacement prefix.

Examples:

$$H_2\overset{N'^1}{N}\text{-}\overset{N^1}{N}H\text{-}\overset{1}{C}O\text{-}\overset{2}{O}\text{-}\overset{3}{C}O\text{-}\overset{N^3}{N}H\text{-}\overset{N'^3}{N}H_2$$

dicarbonic dihydrazide (PIN)
[(hydrazinecarbonyl)oxy]formohydrazide

$$H_2\overset{N'^1}{N}\text{-}\overset{N^1}{N}H\text{-}\overset{1}{C}O\text{-}\overset{2}{N}H\text{-}\overset{3}{C}O\text{-}\overset{N^3}{N}H\text{-}\overset{N'^3}{N}H_2$$

2-imidodicarbonic dihydrazide (PIN)
[(hydrazinecarbonyl)amino]formohydrazide

P-66.3.5.3 Corresponding substituent groups

When a group having priority for citation as a principal characteristic group is present, the hydrazide group is named:

(1) as an acylhydrazinyl compound; the hydrazinyl group is numbered by the numerical locants 1 and 2;

(2) by expressing the corresponding hydrazide substitutively as a prefix by replacing the final letter ‘e’ in the name of the hydrazide by the letter ‘o’.

Method (2) generates preferred IUPAC names.

Examples:

$$OHC-NH-NH-\overset{3}{C}H_2-\overset{2}{C}H_2-\overset{1}{C}OOH$$

3-formohydrazidopropanoic acid (PIN)
3-(2-formylhydrazin-1-yl)propanoic acid

$$H_2N-NH-CO-O-CO-NH-NH-\overset{4}{C}H_2-CH_2-CH_2-\overset{1}{C}OOH$$

4-{[(hydrazinecarbonyl)oxy]formohydrazido}butanoic acid (PIN)
4-(2-{[(hydrazinecarbonyl)oxy]carbonyl}hydrazin-1-yl)butanoic acid

$$H_2N-NH-CO-NH-NH-CH_2-COOH$$

(hydrazinecarbohydrazido)acetic acid (PIN)
[2-(hydrazinecarbonyl)hydrazin-1-yl]acetic acid
[2-(hydrazinylcarbonyl)hydrazin-1-yl]acetic acid

P-66.3.6 Semioxamazones

Semioxamazones have the general structure $R=N-NH-CO-CO-NH_2$. They are derivatives of the hydrazide of oxamic acid. Their preferred IUPAC names are based on the parent name acetamide, but they may also be named as derivatives of oxamic hydrazide.

Example:

$$C_6H_5-CH=N-NH-COCO-NH_2$$

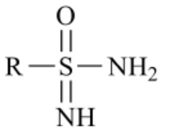
2-(benzylidenehydrazinyl)-2-oxoacetamide (PIN)
N′-benzylideneoxamic hydrazide

P-66.4 AMIDINES, AMIDRAZONES, HYDRAZIDINES, AND AMIDOXIMES (AMIDE OXIMES)

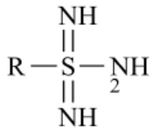
P-66.4.1 Amidines
P-66.4.2 Amidrazones
P-66.4.3 Hydrazidines
P-66.4.4 Amidoximes (amide oximes)

P-66.4.1 Amidines

Compounds having the general structure $R-C(=NH)-NH_2$ generically are known as ‘carboxamidines’ and those having the general structure $R-S(=NH)-NH_2$ as ‘sulfinamidines’. Compounds having the structures below are known only as ‘sulfonimidamides’, and not as amidines.



or



P-66.4.1.1 Suffixes for amidines
P-66.4.1.2 Amidines of carbonic, and di- and polycarbonic acids
P-66.4.1.3 Prefixes for the amidine characteristic group
P-66.4.1.4 Substituted amidines
P-66.4.1.5 Formamidine disulfides
P-66.4.1.6 Diamidides

P-66.4.1.1 Suffixes for amidines

Amidines are named as amides by functional replacement nomenclature in which the =O atom has been replaced by the =NH group. As a principal characteristic group they are designated by the suffixes ‘-imidamide’ and ‘-carboximidamide’. The locant for the $–NH_2$ group is *N* and for the imino group *N*′. The suffixes ‘-amidine’ and ‘-carboxamidine’ are no longer recommended.

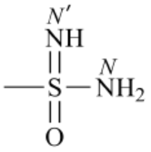
$$–(C)(=\overset{N'}{N}H)-\overset{N}{N}H_2$$

-imidamide (preferred suffix)

$$–C(=\overset{N'}{N}H)-\overset{N}{N}H_2$$

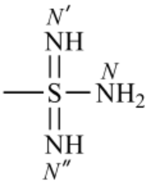
-carboximidamide (preferred suffix)

Suffixes for the sulfonic and sulfinic analogues and their selenium and tellurium analogues are named similarly. For ‘sulfonodiimidamides’ and analogues, the locant for the second ‘imido’ group is *N*″.



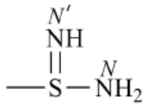
$$-\underset{\underset{\textstyle \mathrm{O}}{\|}}{\overset{\overset{\textstyle \overset{N'}{\mathrm{NH}}}{\|}}{\mathrm{S}}}-\overset{N}{\mathrm{NH}_2}$$

-sulfonimidamide (preselected suffix)



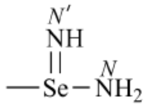
$$-\underset{\underset{\textstyle \underset{N''}{\mathrm{NH}}}{\|}}{\overset{\overset{\textstyle \overset{N'}{\mathrm{NH}}}{\|}}{\mathrm{S}}}-\overset{N}{\mathrm{NH}_2}$$

-sulfonodiimidamide (preselected suffix)



$$-\overset{\overset{\textstyle \overset{N'}{\mathrm{NH}}}{\|}}{\mathrm{S}}-\overset{N}{\mathrm{NH}_2}$$

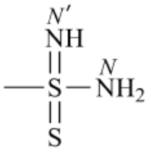
-sulfinimidamide (preselected suffix)



$$-\overset{\overset{\textstyle \overset{N'}{\mathrm{NH}}}{\|}}{\mathrm{Se}}-\overset{N}{\mathrm{NH}_2}$$

-seleninimidamide (preselected suffix)

Suffixes for groups containing S, Se, and Te in place of O in a sulfonimidamide suffix are named by functional replacement, for example:



$$-\underset{\underset{\textstyle \mathrm{S}}{\|}}{\overset{\overset{\textstyle \overset{N'}{\mathrm{NH}}}{\|}}{\mathrm{S}}}-\overset{N}{\mathrm{NH}_2}$$

-sulfonimidothioamide (preselected suffix)

The suffix ‘imidamide’ is used to denote an acyclic amidine with one terminal amidine characteristic group; two terminal amidine characteristic groups on an acyclic parent hydride are denoted by the suffix ‘diimidamide’. All the other suffixes are used to name acyclic polyamidines and all amidines having the suffix attached to a cyclic parent hydride or to a heteroatom of a heteroacyclic parent hydride.

Retained names of amidines are formed by replacing the ‘amide’ ending in names of amides by ‘imidamide’, but these are not preferred IUPAC names; preferred IUPAC names are derived systematically. Other than that, the nomenclatural properties of amides are transferred to amidines; thus, names of amidines correspond to preferred names of amides. Amide names that are not substitutable generate nonsubstitutable amidine names.

Examples:

$$\mathrm{CH_3\text{-}[CH_2]_4\text{-}\overset{1}{C}(=\overset{N'}{N}H)\text{-}\overset{N}{N}H_2}$$

hexanimidamide (PIN)
(no longer hexanamidine)

$$\mathrm{C_6H_{11}\text{-}C(=\overset{N'}{N}H)\text{-}\overset{N}{N}H_2}$$

cyclohexanecarboximidamide (PIN)
(no longer cyclohexanecarboxamidine)

$$\mathrm{\overset{2}{C}H_3\text{-}\overset{1}{C}(=\overset{N'}{N}H)\text{-}\overset{N}{N}H_2}$$

ethanimidamide (PIN)
acetimidamide
(no longer acetamidine)

$$\mathrm{\overset{1}{C}H_3\text{-}S(=\overset{N'}{N}H)\text{-}\overset{N}{N}H_2}$$

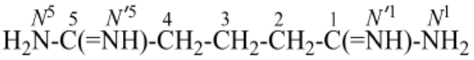
methanesulfinimidamide (PIN)
(no longer methanesulfinamidine)

$$\mathrm{H\overset{1}{C}(=\overset{N'}{N}H)\text{-}\overset{N}{N}H_2}$$

methanimidamide (PIN)

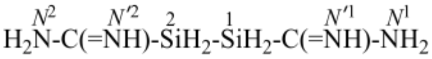
formimidamide
(no longer formamidine)

The letter locants '*N*', '*N*′', etc. with superscripted numbers are used to differentiate among the different nitrogen atoms for 'diimidamides'



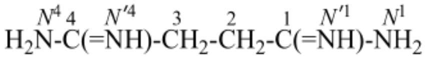
$\overset{N^5}{H_2N}\text{-}\overset{5}{C}(=\overset{N'^5}{N}H)\text{-}\overset{4}{C}H_2\text{-}\overset{3}{C}H_2\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}(=\overset{N'^1}{N}H)\text{-}\overset{N^1}{N}H_2$

pentanediimidamide (PIN)
(no longer pentanediamidine)



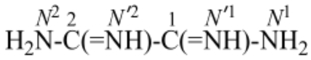
$H_2\overset{N^2}{N}\text{-}C(=\overset{N'^2}{N}H)\text{-}\overset{2}{Si}H_2\text{-}\overset{1}{Si}H_2\text{-}C(=\overset{N'^1}{N}H)\text{-}\overset{N^1}{N}H_2$

disilane-1,2-dicarboximidamide (PIN)
(no longer disilane-1,2-dicarboxamidine)



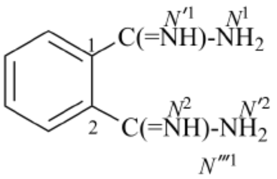
$H_2\overset{N^4}{N}\text{-}\overset{4}{C}(=\overset{N'^4}{N}H)\text{-}\overset{3}{C}H_2\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}(=\overset{N'^1}{N}H)\text{-}\overset{N^1}{N}H_2$

butanediimidamide (PIN)
succinimidamide

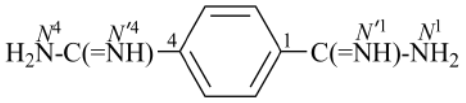


$H_2\overset{N^2}{N}\text{-}\overset{2}{C}(=\overset{N'^2}{N}H)\text{-}\overset{1}{C}(=\overset{N'^1}{N}H)\text{-}\overset{N^1}{N}H_2$

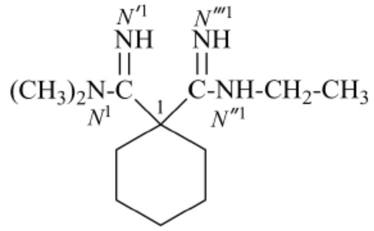
ethanediimidamide (PIN)
oxalimidamide



benzene-1,2-dicarboximidamide (PIN)
phthalimidamide
(no longer benzene-1,2-dicarboxamidine)



benzene-1,4-dicarboximidamide (PIN)
terephthalimidamide
(no longer benzene-1,4-dicarboxamidine)

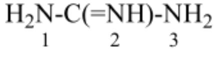


N''^1-ethyl-N^1,N^1-dimethylcyclohexane-1,1-dicarboximidamide (PIN)

P-66.4.1.2 Amidines of carbonic, and di- and polycarbonic acids

P-66.4.1.2.1 Guanidine and its derivatives

P-66.4.1.2.1.1 The preferred IUPAC name for the 'amidine' related to carbonic acid, $H_2N\text{-}C(=NH)\text{-}NH_2$, is the retained name 'guanidine'; the locants *N*, *N*′ and *N*″ are used in preferred IUPAC names. The locants 1, 2, and 3 have been used but are no longer recommended even for general nomenclature.



$H_2\underset{1}{\overset{N}{N}}\text{-}C(=\underset{2}{\overset{N''}{N}}H)\text{-}\underset{3}{\overset{N'}{N}}H_2$

The systematic functional replacement name 'carbonimidic diamide' may be used in general nomenclature.

P-66.4.1.2.1.2 Hydrocarbyl derivatives are named as substituted guanidines. When the position of the double bond is unknown, the preferred IUPAC name uses a minimum number of primes.

Examples:

$(CH_3)_2\overset{N}{N}\text{-}C(=\overset{N''}{N}\text{-}C_6H_5)\text{-}\overset{N'}{N}(CH_3)_2$

N,*N*,*N*′,*N*′-tetramethyl-*N*″-phenylguanidine (PIN)
N,*N*,*N*′,*N*′-tetramethyl-*N*″-phenylcarbonimidic diamide

$CH_3\text{-}\overset{N'}{N}H\text{-}C(=\overset{N''}{N}H)\text{-}\overset{N}{N}(CH_3)_2$

N,*N*,*N*′-trimethylguanidine (PIN)
N,*N*,*N*′-trimethylcarbonimidic diamide

$CH_3\text{-}\overset{N'}{N}H\text{-}C(=\overset{N''}{N}H)\text{-}\overset{N}{N}H\text{-}CH_3$ or $CH_3\text{-}\overset{N'}{N}H\text{-}C(=\overset{N''}{N}\text{-}CH_3)\text{-}\overset{N}{N}H_2$

N,*N*′-dimethylguanidine (PIN)
(not *N*,*N*″-dimethylguanidine)
N,*N*′-dimethylcarbonimidic diamide

P-66.4.1.2.1.3 In the presence of a characteristic group having seniority over guanidine (see item 11 in P-41), the following prefixes are used. The prefix guanidino may be used in general nomenclature.

$H_2\overset{N'}{N}\text{-}C(=\overset{N''}{N}H)\text{-}\overset{N}{N}H\text{–}$

carbamimidoylamino (preferred prefix)
carbamimidamido
[amino(imino)methyl]amino
guanidino

$(H_2N)_2C{=}N\text{–}$

(diaminomethylidene)amino (preferred prefix)

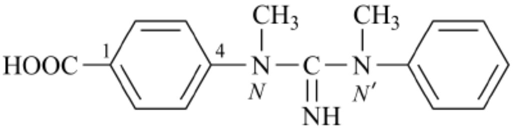
Examples:

$(H_2N)_2C{=}N\text{-}CH_2\text{-}COOH$

N-(diaminomethylidene)glycine
[(diaminomethylidene)amino]acetic acid

$(H_2N)_2C{=}N\text{-}\overset{4}{C}H_2\text{-}CH_2\text{-}CH_2\text{-}\overset{1}{C}OOH$

4-[(diaminomethylidene)amino]butanoic acid (PIN)



4-[methyl(*N*-methyl-*N*-phenylcarbamimidoyl)amino]benzoic acid (PIN)
4-({imino[methyl(phenyl)amino]methyl}methylamino)benzoic acid
4-(*N*,*N*′-dimethyl-*N*′-phenylcarbamimidamido)benzoic acid

$H_2N\text{-}C(=NH)\text{-}NH\text{-}CHO$

N-carbamimidoylformamide (PIN)
N-[amino(imino)methyl]formamide
(not *N*-formylguanidine)

$H_2N\text{-}C(=NH)\text{-}NH\text{-}CO\text{-}NH_2$

N-carbamimidoylurea (PIN)
N-[amino(imino)methyl]urea
(not *N*-carbamoylguanidine)

$H_2N\text{-}C(=NH)\text{-}\overset{N}{N}H\text{-}\overset{1}{C}O\text{-}\overset{2}{C}H_3$

N-carbamimidoylacetamide (PIN)
N-(*C*-aminocarbonimidoyl)acetamide
N-[amino(imino)methyl]acetamide
(not *N*-acetylguanidine)

P-66.4.1.2.2 Condensed guanidines.

The names biguanide, triguanide, etc., are no longer recommended. Condensed guanidines, $H_2N\text{-}[C(=NH)\text{-}NH]_n\text{-}H$ where $n = 2, 3,$ or 4 are named systematically as the diamides of imidodicarbonimidic acid, diimidotricarbonimidic acid, and triimidotetracarbonimidic acid. Locants, as shown, are used to indicate the positions of substituents.

$$\overset{N^1}{\mathrm{H_2N}}\text{-}\overset{1}{\mathrm{C}}(=\overset{N'^1}{\mathrm{NH}})\text{-}\overset{2}{\mathrm{N}}\mathrm{H}\text{-}\overset{3}{\mathrm{C}}(=\overset{N'^3}{\mathrm{NH}})\text{-}\overset{N^3}{\mathrm{N}}\mathrm{H_2}$$

imidodicarbonimidic diamide (PIN)

$$\overset{N^1}{\mathrm{H_2N}}\text{-}\overset{1}{\mathrm{C}}(=\overset{N'^1}{\mathrm{NH}})\text{-}\overset{2}{\mathrm{N}}\mathrm{H}\text{-}\overset{3}{\mathrm{C}}(=\overset{N^3}{\mathrm{NH}})\text{-}\overset{4}{\mathrm{N}}\mathrm{H}\text{-}\overset{5}{\mathrm{C}}(=\overset{N'^5}{\mathrm{NH}})\text{-}\overset{N^5}{\mathrm{N}}\mathrm{H_2}$$

diimidotricarbonimidic diamide (PIN)

Example:

$$\overset{N^3}{\mathrm{H_2N}}\text{-}\overset{3}{\mathrm{C}}(=\overset{N'^3}{\mathrm{NH}})\text{-}\overset{2}{\mathrm{N}}\mathrm{H}\text{-}\overset{1}{\mathrm{C}}(=\overset{N'^1}{\mathrm{N}}\text{-}\mathrm{CH_2}\text{-}\mathrm{CH_3})\text{-}\overset{N^1}{\mathrm{N}}(\mathrm{C_6H_5})_2$$

N'^1-ethyl-N^1,N^1-diphenylimidodicarbonimidic diamide (PIN)

For polyguanides, where *n* = 5 and higher, skeletal replacement ('a') nomenclature leads to preferred IUPAC names

Example:

$$\mathrm{H_2N}\text{-}\overset{1}{\mathrm{C}}(=\mathrm{NH})\text{-}\overset{2}{\mathrm{N}}\mathrm{H}\text{-}\overset{3}{\mathrm{C}}(=\mathrm{NH})\text{-}\overset{4}{\mathrm{N}}\mathrm{H}\text{-}\overset{5}{\mathrm{C}}(=\mathrm{NH})\text{-}\overset{6}{\mathrm{N}}\mathrm{H}\text{-}\overset{7}{\mathrm{C}}(=\mathrm{NH})\text{-}\overset{8}{\mathrm{N}}\mathrm{H}\text{-}\overset{9}{\mathrm{C}}(=\mathrm{NH})\text{-}\mathrm{NH_2}$$

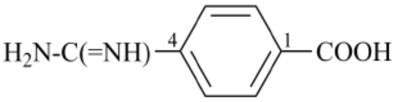
3,5,7-triimino-2,4,6,8-tetraazanonane-1,9-diimidamide (PIN)

P-66.4.1.3 Prefixes for the amidine characteristic group

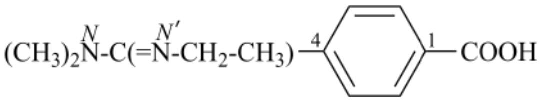
P-66.4.1.3.1 The systematic name for the group –C(=NH)-NH_2 is 'carbamimidoyl'; it is the name of the acyl group derived from the name carbamimidic acid, HO-C(=NH)-NH_2 and is the preferred IUPAC prefix. The prefix 'amidino' is no longer recommended. In the acyl group, the –NH_2 group is denoted by the locant *N* and the =NH group by *N*′.

The prefix 'amidino' is no longer acceptable in IUPAC nomenclature; 'carbamimidoyl' is now recommended for preferred IUPAC names.

Examples:



4-carbamimidoylbenzoic acid (PIN)
4-[amino(imino)methyl]benzoic acid
(not 4-amidinobenzoic acid)



4-(*N*′-ethyl-*N*,*N*-dimethylcarbamimidoyl)benzoic acid (PIN)
4-[(dimethylamino)(ethylimino)methyl]benzoic acid
[not 4-(*N*′-ethyl-*N*,*N*-dimethylamidino)benzoic acid]

P-66.4.1.3.2 When the carbon atom of the H_2N-C(=NH)– group terminates a chain, the groups –NH_2 and =NH are designated by the prefixes 'amino' and 'imino', respectively.

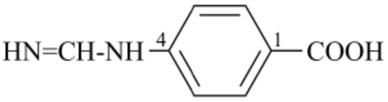
Example:

$$(\mathrm{CH_3})_2\mathrm{N}\text{-}\overset{4}{\mathrm{C}}(=\mathrm{N}\text{-}\mathrm{CH_2}\text{-}\mathrm{CH_3})\text{-}\overset{3}{\mathrm{C}}\mathrm{H_2}\text{-}\overset{2}{\mathrm{C}}\mathrm{H_2}\text{-}\overset{1}{\mathrm{C}}\mathrm{O}\text{-}\mathrm{O}\text{-}\mathrm{CH_3}$$

methyl 4-(dimethylamino)-4-(ethylimino)butanoate (PIN)
(not methyl 3-[*C*-(dimethylamino)-*N*-ethylcarbonimidoyl]propanoate)
(not methyl 3-(N^2-ethyl-N^1,N^1-dimethylamidino)propionate)

P-66.4.1.3.3 The substituent group HN=CH-NH– is named 'methanimidamido'; it can also be named as a compound substituent prefix 'formimidoylamino' or a complex substituent prefix '(iminomethyl)amino'. 'Methanimidamido' is the preferred IUPAC prefix. The substituent group H_2N-CH=N– can only be named as a complex substituent group, '(aminomethylidene)amino'.

Example:



4-methanimidamidobenzoic acid (PIN)
4-[(iminomethyl)amino]benzoic acid
4-(formimidoylamino)benzoic acid

P-66.4.1.3.4 Substituent prefixes corresponding to the suffixes sulfonimidamide, sulfinimidamide, and related selenium and tellurium suffixes are formed systematically by concatenation using the prefix 'amino-' and the name of the appropriate acyl group:

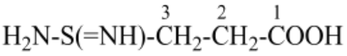
$-S(O)(=NH)\text{-}NH_2$
S-aminosulfonimidoyl (preselected prefix)

$-S(=NH)_2\text{-}NH_2$
S-aminosulfonodiimidoyl (preselected prefix)

$-S(=NH)\text{-}NH_2$
S-aminosulfinimidoyl (preselected prefix)

Note: The italic letter locant '*S*' is used to avoid potential ambiguity regarding substitution on the imido nitrogen atom

Example:



$H_2N\text{-}S(=NH)\text{-}\overset{3}{C}H_2\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}OOH$

3-(*S*-aminosulfinimidoyl)propanoic acid (PIN)

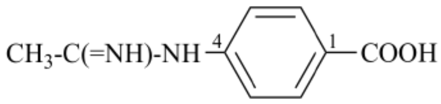
P-66.4.1.3.5 In the presence of a characteristic group cited as a suffix, the group R-C(=NH)NH– or R-S(O)(=NH)NH– and their selenium and tellurium analogues are named in two ways.

(1) substitutively, by using a prefix formed by changing the final letter 'e' in the complete name of the amide to 'o', thus changing the suffixes 'imidamide' and 'carboximidamide' into 'imidamido' and 'carboximidamido', respectively, or 'sulfonimidamide' to 'sulfonimidamido', etc.

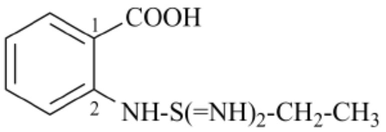
(2) substitutively, by using 'acylamino' prefixes formed by substituting the name of the acyl group to the substituent 'amino'

Method (1) generates preferred IUPAC prefixes.

Examples:



4-ethanimidamidobenzoic acid (PIN)
4-(acetimidoylamino)benzoic acid
4-acetimidamidobenzoic acid



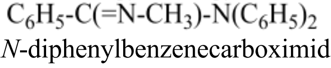
2-(ethanesulfonodiimidamido)benzoic acid (PIN)
2-(ethanesulfonodiimidoylamino)benzoic acid

P-66.4.1.4 Substituted amidines

P-66.4.1.4.1 *N*-Substituted amidines are named by prefixing the name of the appropriate substituent to the name of the unsubstituted imidamides, with *N* and *N*′ as locants when there is only one imidamide suffix; the locant *N* refers to the amino group and *N*′ refers to the imino group. The locants *N* and *N*′ with superscripted numbers for example, N^1 or N'^2, are used when there are two or more imidamide suffixes. Because of tautomerism, the locants *N*, *N*′, etc. are used when only one substituent is present on each imidamide group.

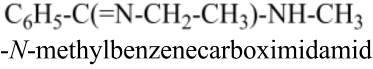
The locants *N* and *N*′ are used for the NH_2 and NH group of amidines, respectively, rather than the locants N^1 and N^2 which were used in the 1979 recommendations (ref. 1).

Examples:



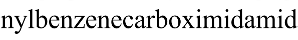
$C_6H_5\text{-}C(=\overset{N'}{N}\text{-}CH_3)\text{-}\overset{N}{N}(C_6H_5)_2$

N′-methyl-*N*,*N*-diphenylbenzenecarboximidamide (PIN)
(not *N*′-methyl-*N*,*N*-diphenylbenzenecarboxamidine)



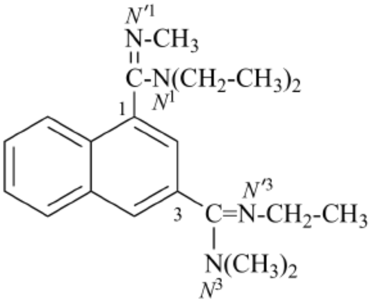
$C_6H_5\text{-}C(=\overset{N'}{N}\text{-}CH_2\text{-}CH_3)\text{-}\overset{N}{N}H\text{-}CH_3$

N′-ethyl-*N*-methylbenzenecarboximidamide (PIN)
(not *N*′-ethyl-*N*-methylbenzenecarboxamidine)



$C_6H_5\text{-}C(=\overset{N'}{N}H)\text{-}\overset{N}{N}H\text{-}C_6H_5$

N-phenylbenzenecarboximidamide (PIN)
(not *N*-phenylbenzenecarboxamidine;
not benzimidanilide)

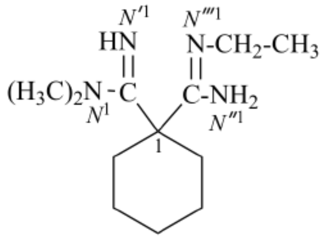


N^1,N^1,N'^3-triethyl-N'^1,N^3,N^3-trimethylnaphthalene-1,3-dicarboximidamide (PIN)

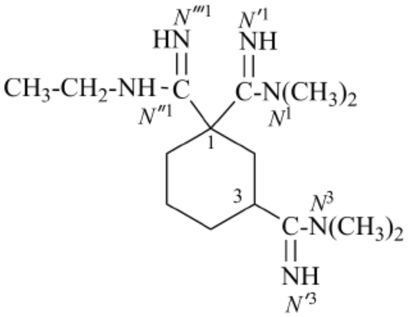
P-66.4.1.4.2 Geminal carboxamidine groups

When geminal carboxamidine groups are present, the locants *N*, *N*′, *N*″, *N*‴ are used. Lowest locants are assigned to the most substituted group; when there is a choice, lowest locants are assigned to the first cited *N*-substituent. For polyamidines with at least one pair of geminal amidine groups, superscripted numerical locants indicating the position of the amidine group on a chain or cycle are used. This system of *N*-locants in association with superscript numerical locants is also recommended for naming disubstituted amines (see P-62.2.4.1) and disubstituted amides (see P-66.1.1.3.1.2).

Examples:



N'''^1-ethyl-N^1,N^1-dimethylcyclohexane-1,1-dicarboximidamide (PIN)

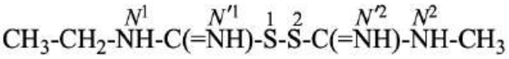


N''^1-ethyl-N^1,N^1,N^3,N^3-tetramethylcyclohexane-1,1,3-tricarboximidamide (PIN)

P-66.4.1.5 Formamidine disulfides

The compound $H_2N\text{-}C(=NH)\text{-}S\text{-}S\text{-}C(=NH)\text{-}NH_2$ and its derivatives have been named previously on the basis of the parent structure ‘formamidine disulfide’. They are now named on the basis of the parent compound ‘dicarbonic acid’ or as a dithioperoxyanhydride which is the preferred IUPAC name.

Example:

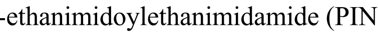

$CH_3\text{-}CH_2\text{-}\overset{N^1}{NH}\text{-}C(=\overset{N'^1}{NH})\text{-}\overset{1}{S}\text{-}\overset{2}{S}\text{-}C(=\overset{N'^2}{NH})\text{-}\overset{N^2}{NH}\text{-}CH_3$

N-ethylcarbamimidic *N*-methylcarbamimidic dithioperoxyanhydride (PIN)
[not N^1-ethyl-N^2-methyldisulfanedicarboximidamide (numbering shown);
not *N*-ethyl-*N*″-methyl(dithioperoxy)dicarbonimidic diamide;
not N^1-ethyl-N^3-methyl-α,α′-dithiobisformamidine (see C-951.5 in ref. 1)]
Note: The anhydride is the higher class in seniority (see P-41).

P-66.4.1.6 Diamidides

Diamidides are analogues of acyclic carboxylic anhydrides in which the =O atoms have been replaced by =NR groups and the anhydride oxygen atom by –NR– giving the general formula R-C(=NR′)-N(R″)-C(=NR‴)-R‴′. Preferred IUPAC names are formed systematically as *N*-imidoylimidamides.

Example:


$CH_3\text{-}C(=NH)\text{-}\overset{N}{NH}\text{-}\overset{1}{C}(=\overset{N'}{NH})\text{-}CH_3$

N-ethanimidoylethanimidamide (PIN)

N-acetimidoylacetimidamide
N-(1-iminoethyl)ethanimidamide

P-66.4.2 Amidrazones

P-66.4.2.1 Amidrazone suffixes

Compounds having the general structure $\mathrm{R{-}C(NH_2){=}N{-}NH_2}$ or the tautomeric structure $\mathrm{R{-}C({=}NH){-}NH{-}NH_2}$ have the class name 'amidrazones' and are named substitutively using the suffixes 'hydrazonamide' or 'carbohydrazonamide', and 'imidohydrazide' or 'carboximidohydrazide', respectively. *N*-Substitution, when the position of the double bond is known, is designated with the following locants:

for carbohydrazonamides $\mathrm{R{-}C({=}N{-}}\overset{N'}{\mathrm{N}}\mathrm{H_2){-}}\overset{N}{\mathrm{N}}\mathrm{H_2}$

for carboximidohydrazides $\mathrm{R{-}C({=}}\overset{N''}{\mathrm{N}}\mathrm{H){-}}\overset{N}{\mathrm{N}}\mathrm{H{-}}\overset{N'}{\mathrm{N}}\mathrm{H_2}$

Preferred IUPAC names use the locants *N*, *N*′, and *N*″ as shown. The previous methods of naming amidrazones as 'amide hydrazones' or 'hydrazide imides', or as amidrazones when the structure is not known, are no longer recommended.

When the position of the double bond is unknown, the senior characteristic group, carbohydrazonamide, is chosen to denote the tautomeric structure, with appropriate locants *N* and *N*′ to denote substitution. When the position of the substituted suffixes must be indicated in a name, locants designating the positions of the suffixes are superscripted to the appropriate *N* locants.

Retained names of amidrazones are formed by replacing the 'amide' ending in names of amides by 'ohydrazonamide' and are only used in general nomenclature. Preferred IUPAC names of amidrazones are formed systematically. Otherwise, the nomenclatural properties of amides are transferred to amidrazones; thus, preferred names of amidrazones correspond to preferred names of amides; and amides that are not substitutable generate nonsubstitutable amidrazones.

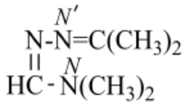
Examples:

$$\mathrm{CH_3{-}C({=}N{-}}\overset{N'}{\mathrm{N}}\mathrm{H_2){-}}\overset{N}{\mathrm{N}}\mathrm{H_2}$$
ethanehydrazonamide (PIN)

$$\mathrm{C_6H_5{-}C({=}N{-}}\overset{N'}{\mathrm{N}}\mathrm{H_2){-}}\overset{N}{\mathrm{N}}\mathrm{H_2}$$
benzenecarbohydrazonamide (PIN)

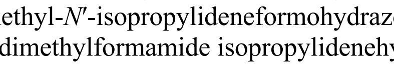
$$\mathrm{H{-}C({=}}\overset{N''}{\mathrm{N}}\mathrm{H){-}}\overset{N}{\mathrm{N}}\mathrm{H{-}}\overset{N'}{\mathrm{N}}\mathrm{H_2}$$
methanimidohydrazide (PIN)

$$\mathrm{C_6H_{11}{-}C({=}}\overset{N''}{\mathrm{N}}\mathrm{H){-}}\overset{N}{\mathrm{N}}\mathrm{H{-}}\overset{N'}{\mathrm{N}}\mathrm{H_2}$$
cyclohexanecarboximidohydrazide (PIN)



$$\begin{array}{l} \overset{N'}{\mathrm{N}}\mathrm{{-}N{=}C(CH_3)_2} \\ \| \\ \mathrm{HC{-}}\overset{N}{\mathrm{N}}\mathrm{(CH_3)_2} \end{array}$$

N,*N*-dimethyl-*N*′-(propan-2-ylidene)methanehydrazonamide (PIN)
N,*N*-dimethyl-*N*′-isopropylideneformohydrazonamide
(not *N*,*N*-dimethylformamide isopropylidenehydrazone)



$$\mathrm{CH_3{-}CH_2{-}}\overset{N''}{\mathrm{N}}{=}\overset{\mathrm{C_6H_5}}{\mathrm{C}}\mathrm{{-}}\overset{N}{\mathrm{N}}\mathrm{(CH_3){-}}\overset{N'}{\mathrm{N}}\mathrm{H{-}C_6H_5}$$

N″-ethyl-*N*-methyl-*N*′-phenylbenzenecarboximidohydrazide (PIN)
N″-ethyl-*N*-methyl-*N*′-phenylbenzimidohydrazide
(not N^1-methyl-N^2-phenylbenzohydrazide ethylimide)

$$\mathrm{H_2}\overset{N'^1}{\mathrm{N}}\mathrm{{-}}\overset{N^1}{\mathrm{N}}\mathrm{H{-}}\overset{1}{\mathrm{C}}\mathrm{({=}}\overset{N''^1}{\mathrm{N}}\mathrm{H){-}}\overset{2}{\mathrm{C}}\mathrm{({=}}\overset{N''^2}{\mathrm{N}}\mathrm{H){-}}\overset{N^2}{\mathrm{N}}\mathrm{H{-}}\overset{N'^2}{\mathrm{N}}\mathrm{H_2}$$
ethanediimidohydrazide (PIN)

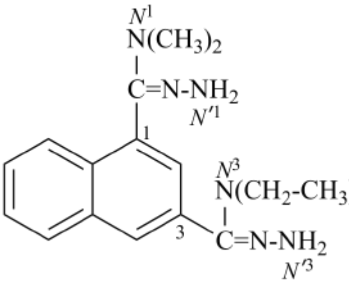
$$\mathrm{H_2}\overset{N^1}{\mathrm{N}}\mathrm{{-}}\overset{1}{\mathrm{C}}\mathrm{({=}N{-}}\overset{N'^1}{\mathrm{N}}\mathrm{H_2){-}}\overset{2}{\mathrm{C}}\mathrm{({=}N{-}}\overset{N'^2}{\mathrm{N}}\mathrm{H_2){-}}\overset{N^2}{\mathrm{N}}\mathrm{H_2}$$
ethanedihydrazonamide (PIN)

$$H_2N\text{-}NH\text{-}\overset{2}{C}(=NH)\text{-}\overset{1}{C}(=N\text{-}NH_2)\text{-}NH_2$$

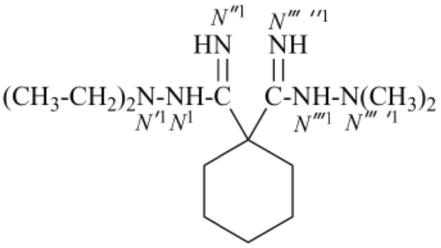
2-hydrazinyl-2-iminoethanehydrazonamide (PIN)

$$H_2N\text{-}C(=NH)\text{-}\overset{1}{N}H\text{-}\overset{2}{N}H\text{-}\overset{3}{N}=\overset{4}{N}\text{-}C(=NH)\text{-}\overset{1}{N}H\text{-}\overset{2}{N}H\text{-}NO$$

4-(2-nitrosohydrazine-1-carboximidoyl)tetraaz-3-ene-1-carboximidamide (PIN)
[an imidamide (an amidine) is senior to an imidohydrazide (an amidrazone)]



N^3,N^3-diethyl-N^1,N^1-dimethylnaphthalene-1,3-dicarbohydrazonamide (PIN)


N''^1
$N'''\,''^1$
HN
NH
$(CH_3\text{-}CH_2)_2N\text{-}NH\text{-}C$
$C\text{-}NH\text{-}N(CH_3)_2$
N'^1 N^1
N'''^1 $N'''\,'^1$

N'^1,N'^1-diethyl-$N'''\,'^1$,$N'''\,'^1$-dimethylcyclohexane-1,1-dicarboximidohydrazide (PIN)
Note: For locants *N*, *N*′, etc. in association with numerical locants, see P-16.9, P-62.2.4.1.2 and P-66.4.1.4.2)

Amidrazones derived from sulfonic acid, sulfinic acid, and related acids, are named in accordance with the same principles.

Example:

$$C_6H_5\text{-}S(=NNH_2)\text{-}NH_2$$

benzenesulfinohydrazonamide (PIN)

P-66.4.2.2 Amidrazones of carbonic acid and di- and polycarbonic acids

The general methodology discussed in P-65.2 is applied to generate the names for amidrazones derived from carbonic, di-, and polycarbonic acids.

Examples:

$$\overset{2}{H_2N}\text{-}\overset{1}{N}H\text{-}C(=\overset{N''}{N}H)\text{-}\overset{N}{N}H\text{-}\overset{N'}{N}H_2$$

hydrazinecarboximidohydrazide (PIN)
carbonimidic dihydrazide

$$\overset{N}{H_2N}\text{-}C(=N\text{-}\overset{N''}{N}H_2)\text{-}\overset{N'}{N}H_2$$

carbonohydrazonic diamide (PIN)

$$\overset{N'^1}{H_2N}\text{-}\overset{N^1}{N}H\text{-}\overset{1}{C}(=\overset{N''^1}{N}H)\text{-}\overset{2}{O}\text{-}\overset{3}{C}(=\overset{N''^3}{N}H)\text{-}\overset{N^3}{N}H\text{-}\overset{N'^3}{N}H_2$$

dicarbonimidic dihydrazide (PIN; see P-65.2.3.1)
(not 1,3-diimidodicarbonic dihydrazide)

$$\overset{N^1}{H_2N}\text{-}\overset{1}{C}(=N\text{-}\overset{N'^1}{N}H_2)\text{-}\overset{2}{O}\text{-}\overset{3}{C}(=N\text{-}\overset{N'^3}{N}H_2)\text{-}\overset{N^3}{N}H_2$$

dicarbonohydrazonic diamide (PIN; see P-65.2.3.1)
(not 1,3-dihydrazonodicarbonic diamide)

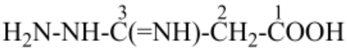
$$H_2N\text{-}NH\text{-}C(=NH)\text{-}O\text{-}C(=N\text{-}\overset{N}{N}H_2)\text{-}\overset{N'}{N}H_2$$

[(hydrazinecarboximidoyl)oxy]methanehydrazonamide (PIN)
[(carbamohydrazonoyl)oxy]methanimidohydrazide
[not [(hydrazinecarboximidoyl)oxy]formohydrazonamide]

P-66.4.2.3 Amidrazone prefixes

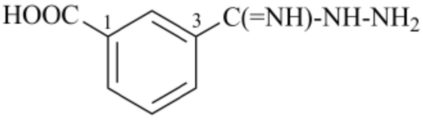
P-66.4.2.3.1 Prefixes for the group –C(=NH)-NHNH$_2$ are ‘hydrazinecarboximidoyl’ (preferred prefix) derived from hydrazinecarboximidic acid, and ‘carbonohydrazidimidoyl’, derived from carbonohydrazidimidic acid. When this group is located at the end of a carbon chain, the prefixes ‘imino’ and ‘hydrazinyl’ are used in preferred IUPAC names in order to avoid fragmenting the parent chain.

Examples:



$H_2N\text{-}NH\text{-}\overset{3}{C}(=NH)\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}OOH$

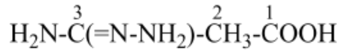
3-hydrazinyl-3-iminopropanoic acid (PIN)
(hydrazinecarboximidoyl)acetic acid
carbonohydrazidimidoylacetic acid
(*C*-hydrazinylcarbonimidoyl)acetic acid



3-(hydrazinecarboximidoyl)benzoic acid (PIN)
3-carbonohydrazidimidoylbenzoic acid
3-[hydrazinyl(imino)methyl]benzoic acid
3-(*C*-hydrazinylcarbonimidoyl)benzoic acid

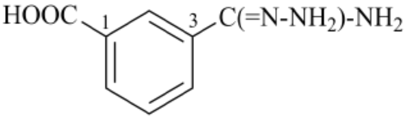
P-66.4.2.3.2 The preferred prefix for the group –C(=N-NH$_2$)-NH$_2$ is ‘carbamohydrazonoyl’. When this group is located at the end of a carbon chain, the prefixes ‘amino’ and ‘hydrazinylidene’ are used in preferred IUPAC names in order to avoid fragmenting the parent chain.

Examples:



$H_2N\text{-}\overset{3}{C}(=N\text{-}NH_2)\text{-}\overset{2}{C}H_3\text{-}\overset{1}{C}OOH$

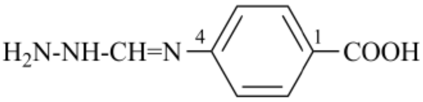
3-amino-3-hydrazinylidenepropanoic acid (PIN)
carbamohydrazonoylacetic acid



3-carbamohydrazonoylbenzoic acid (PIN)
3-[amino(hydrazinylidene)methyl]benzoic acid

P-66.4.2.3.3 Prefixes for the group –NH-CH=N-NH$_2$ are ‘methanehydrazonamido’ (preferred prefix) and ‘(hydrazinylidenemethyl)amino’ and ‘(methanehydrazonoyl)amino’. The preferred prefix for –N=CH-NH-NH$_2$ is ‘(hydrazinylmethylidene)amino’.

Examples:

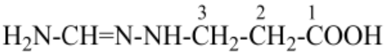


4-[(hydrazinylmethylidene)amino]benzoic acid (PIN)

$H_2N\text{-}N=CH\text{-}NH\text{-}CH_2\text{-}CH_2\text{-}CN$
N-(2-cyanoethyl)methanehydrazonamide (PIN)
(not 3-[(methanehydrazonoyl)amino]propanenitrile;
nor 3-[(hydrazinylidenemethyl)amino]propanenitrile)

P-66.4.2.3.4 The preferred prefix for the group H$_2$N-CH=N-NH– is ‘(aminomethylidene)hydrazinyl’. Prefixes for the group HN=CH-NH-NH– are ‘methanimidohydrazido’ (preferred prefix) and ‘2-(methanimidoyl)hydrazin-1-yl’ and ‘2-(iminomethyl)hydrazin-1-yl’. Prefixes for the group HC(=NNH$_2$)-NH– are ‘methanehydrazonamido’ (preferred prefix) and ‘(methanehydrazonoyl)amino’.

Example:



$H_2N\text{-}CH=N\text{-}NH\text{-}\overset{3}{C}H_2\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}OOH$

3-[2-(aminomethylidene)hydrazin-1-yl]propanoic acid (PIN)

P-66.4.2.3.5 When a group having preference for citation as a principal characteristic group is present, the groups R-C(=N-NH$_2$)-NH– and R-S(O)(=N-NH$_2$)-NH– (and the selenium and tellurium analogues) are named in two ways:

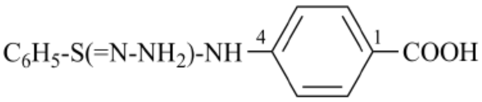
(1) substitutively, by using a prefix formed by changing the final letter ‘e’ in the complete name of the amide to ‘o’;

(2) substitutively, by using ‘acylamino’ prefixes formed by substituting the name of the acyl group to the substituent ‘amino’

Method (1) generates preferred prefixes.

Example:

CH_3-C(=N-NH_2)-NH-CH_2-CH_2-COOH
3-(ethanehydrazonamido)propanoic acid (PIN)
3-[(ethanehydrazonoyl)amino]propanoic acid



4-(benzenesulfinohydrazonamido)benzoic acid (PIN)
4-[(benzenesulfinohydrazonoyl)amino]benzoic acid

P-66.4.2.3.6 When a group having priority for citation as a principal characteristic group is present, a hydrazide group of the type R-C(=NH)-NHNH– or R-S(=NH)$_2$-NHNH– (or the analogous selenium and tellurium group) is named:

(1) by expressing the corresponding hydrazide as a prefix by replacing the final letter ‘e’ in the name of the hydrazide by the letter ‘o’:

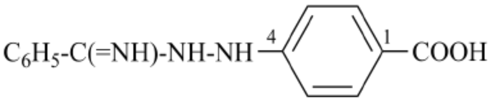
(2) as an acylhydrazinyl prefix; the hydrazinyl group is numbered by using the numerical locants 1 and 2.

Method (1) generates preferred prefixes.

Examples:

HN=CH-NH-NH-CH_2-CH_2-COOH
3-(methanimidohydrazido)propanoic acid (PIN)
3-(2-methanimidoylhydrazin-1-yl)propanoic acid

CH_3-C(=NH)-NH-NH-CH_2-CO-O-CH_3
methyl (ethanimidohydrazido)acetate (PIN)
methyl [2-(ethanimidoyl)hydrazin-1-yl]acetate



(1) 4-(benzenecarboximidohydrazido)benzoic acid (PIN)
(2) 4-[2-(benzenecarboximidoyl)hydrazin-1-yl]benzoic acid

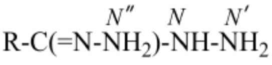
P-66.4.3 Hydrazidines

P-66.4.3.1 Hydrazidine suffixes

Compounds with the general structure R-C(=N-NH_2)-NH-NH_2 have the class name ‘hydrazidines’ and are named substitutively by using the suffixes ‘hydrazonohydrazide’ and ‘carbohydrazonohydrazide’ as prescribed for hydrazides. The former method of naming hydrazidines as hydrazones of the corresponding hydrazides (see C-954.2 in ref. 1) is no longer recommended.

Hydrazidines are named systematically in these recommendations rather than as hydrazones of the corresponding hydrazides as in the 1979 recommendations.

Locants are assigned to nitrogen atoms as follows:

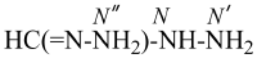


$$\text{R-C(=N-}\overset{N''}{\text{NH}_2}\text{)-}\overset{N}{\text{NH}}\text{-}\overset{N'}{\text{NH}_2}$$

When necessary, the locant indicating the position of the hydrazidine characteristic group on the parent structure is given as a superscript arabic number to the appropriate ‘*N*’ locant.

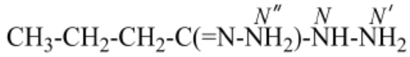
Names of hydrazidines formally derived from carboxylic acids having retained names, formed by replacing the ‘ohydrazide’ ending in names of hydrazides by ‘hydrazonohydrazide’, may be used in general nomenclature. Preferred IUPAC names are formed systematically. Otherwise, the nomenclatural properties of hydrazides are transferred to hydrazidines; thus, preferred names of hydrazidines correspond to preferred names of hydrazides, and hydrazides that are not substitutable generate nonsubstitutable hydrazidines.

Examples:



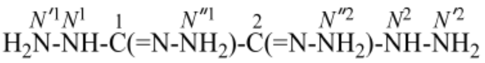
$$\mathrm{HC(=N\text{-}}\overset{N''}{\mathrm{NH_2}}\mathrm{)\text{-}}\overset{N}{\mathrm{NH}}\text{-}\overset{N'}{\mathrm{NH_2}}$$

methanehydrazonohydrazide (PIN)



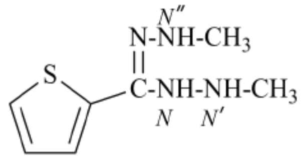
$$\mathrm{CH_3\text{-}CH_2\text{-}CH_2\text{-}C(=N\text{-}}\overset{N''}{\mathrm{NH_2}}\mathrm{)\text{-}}\overset{N}{\mathrm{NH}}\text{-}\overset{N'}{\mathrm{NH_2}}$$

butanehydrazonohydrazide (PIN)

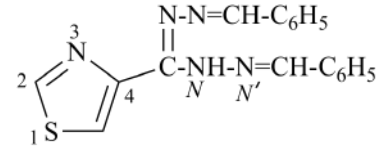


$$\overset{N'^{1}}{\mathrm{H_2N}}\text{-}\overset{N^{1}}{\mathrm{NH}}\text{-}\overset{1}{\mathrm{C}}\mathrm{(=N\text{-}}\overset{N''^{1}}{\mathrm{NH_2}}\mathrm{)\text{-}}\overset{2}{\mathrm{C}}\mathrm{(=N\text{-}}\overset{N''^{2}}{\mathrm{NH_2}}\mathrm{)\text{-}}\overset{N^{2}}{\mathrm{NH}}\text{-}\overset{N'^{2}}{\mathrm{NH_2}}$$

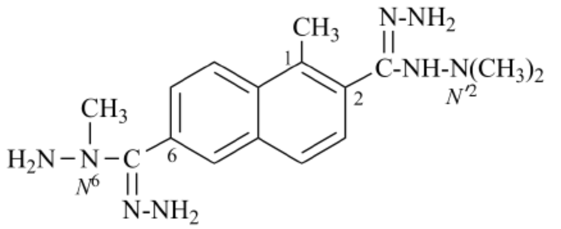
ethanedihydrazonohydrazide (PIN)



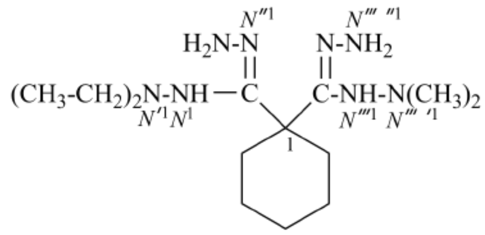
N',N''-dimethylthiophene-2-carbohydrazonohydrazide (PIN)



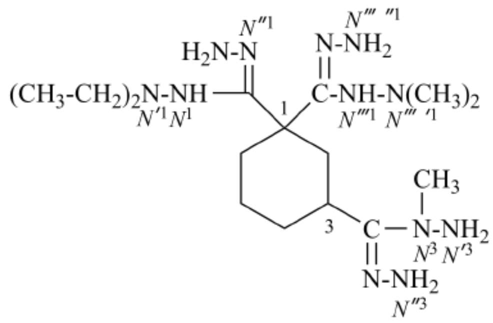
N',N''-dibenzylidene-1,3-thiazole-4-carbohydrazonohydrazide (PIN)



N'^{2}, N'^{2}, N^{6},1-tetramethylnaphthalene-2,6-dicarbohydrazonohydrazide (PIN)



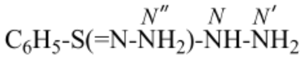
N'^{1},N'^{1}-diethyl-$N'''\,'^{1}$,$N'''\,'^{1}$-dimethylcyclohexane-1,1-dicarbohydrazonohydrazide (PIN)



N'^{1}, N'^{1}-diethyl-$N'''\,'^{1}$,$N'''\,'^{1}$,N^{3}-trimethylcyclohexane-1,1,3-tricarbohydrazonohydrazide (PIN)
(for locants N, N', etc. in association with numerical locants,
see P-16.9, P-62.2.4.1.2, P-66.3.1.2, P-66.3.3, P-66.4.1.1, P-66.4.1.4, and P-66.4.2.1)

P-66.4.3.2 Hydrazidines derived from sulfonic and sulfinic acids, and similar selenium and tellurium acids, are named in accordance with the same principles.

Example:

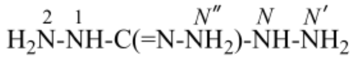


$$\mathrm{C_6H_5\text{-}S(=N\text{-}}\overset{N''}{\mathrm{NH_2}}\mathrm{)\text{-}}\overset{N}{\mathrm{NH}}\text{-}\overset{N'}{\mathrm{NH_2}}$$

benzenesulfinohydrazonohydrazide (PIN)

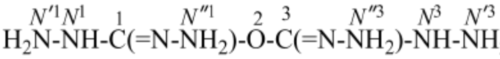
P-66.4.3.3 Hydrazidines derived from carbonic acid and di- and polycarbonic acids follow the procedure for the corresponding hydrazides given above (see P-66.3.5).

Examples:



$H_2\overset{2}{N}\text{-}\overset{1}{N}H\text{-}C(=N\text{-}\overset{N''}{N}H_2)\text{-}\overset{N}{N}H\text{-}\overset{N'}{N}H_2$

hydrazinecarbohydrazonohydrazide (PIN)
carbonohydrazonic dihydrazide (P-65.2.1.3)



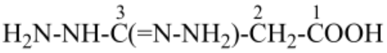
$H_2\overset{N'^1}{N}\text{-}\overset{N^1}{N}H\text{-}\overset{1}{C}(=N\text{-}\overset{N''^1}{N}H_2)\text{-}\overset{2}{O}\text{-}\overset{3}{C}(=N\text{-}\overset{N''^3}{N}H_2)\text{-}\overset{N^3}{N}H\text{-}\overset{N'^3}{N}H_2$

dicarbonohydrazonic dihydrazide (PIN, P-65.2.1.3)
(not dihydrazonodicarbonic dihydrazide)

P-66.4.3.4 Hydrazidine prefixes

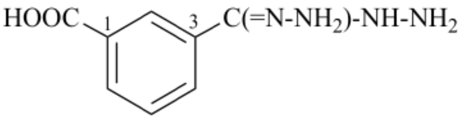
P-66.4.3.4.1 In the presence of a senior characteristic group, the prefixes for the group $–C(=N\text{-}NH_2)\text{-}NH\text{-}NH_2$ are ‘hydrazinecarbohydrazonoyl’ (preferred prefix) or ‘*C*-hydrazinylcarbonohydrazonoyl’. When this group is located at the end of a carbon chain, the prefixes ‘hydrazinyl’ and ‘hydrazinylidene’ are preferred in order to avoid fragmenting the chain.

Examples:

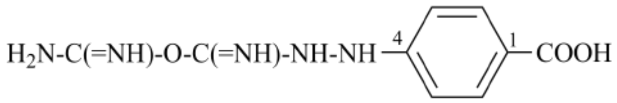


$H_2N\text{-}NH\text{-}\overset{3}{C}(=N\text{-}NH_2)\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}OOH$

3-hydrazinyl-3-hydrazinylidenepropanoic acid (PIN)
(hydrazinecarbohydrazonoyl)acetic acid
(*C*-hydrazinylcarbonohydrazonoyl)acetic acid



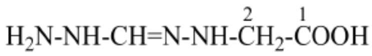
3-(hydrazinecarbohydrazonoyl)benzoic acid (PIN)
3-(*C*-hydrazinylcarbonohydrazonoyl)benzoic acid
3-[hydrazinyl(hydrazinylidene)methyl]benzoic acid



4-[*C*-(carbamimidoyloxy)methanimidohydrazido]benzoic acid (PIN)
4-{2-[*C*-(carbamimidoyloxy)methanimidoyl]hydrazin-1-yl}benzoic acid

P-66.4.3.4.2 In the presence of a senior characteristic group, the names for the group $–NH\text{-}NH\text{-}CH=N\text{-}NH_2$ are ‘2-(hydrazinylidenemethyl)hydrazin-1-yl’ or ‘2-(methanehydrazonoyl)hydrazin-1-yl’ (preferred prefix); and the name for the group $–NH\text{-}N=CH\text{-}NH\text{-}NH_2$ is ‘(hydrazinylmethylidene)hydrazinyl’ (preferred prefix).

Example:



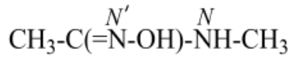
$H_2N\text{-}NH\text{-}CH=N\text{-}NH\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}OOH$

[(hydrazinylmethylidene)hydrazinyl]acetic acid (PIN)

P-66.4.4 Amidoximes (amide oximes)

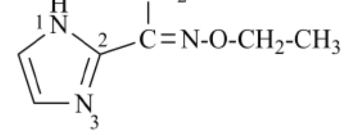
Amide oximes are formally oximes of carboxamides, i.e., compounds having the general structure $R\text{-}C(=N\text{-}OH)\text{-}NH_2$ and derivatives formed by substitution. Preferred IUPAC names are *N*′-hydroxy or *N*′-(alkyloxy) derivatives of carboximidamides (amidines). Suffixes such as ‘amide oxime’ or ‘carboxamide oxime’ are no longer recommended.

Examples:



$CH_3\text{-}C(=\overset{N'}{N}\text{-}OH)\text{-}\overset{N}{N}H\text{-}CH_3$

N′-hydroxy-*N*-methylethanimidamide (PIN)
N′-hydroxy-*N*-methylacetimidamide
(not *N*-methylacetamide oxime)



N′-ethoxy-1*H*-imidazole-2-carboximidamide (PIN)
(not imidazole-2-carboxamide *O*-ethyloxime)

P-66.5 NITRILES

P-66.5.0 Introduction
P-66.5.1 Nomenclature for generating preferred names for nitriles
P-66.5.2 Substituted nitriles
P-66.5.3 Nitriles/cyanides corresponding to carbonic and di- and polycarbonic acids
P-66.5.4 Nitrile oxides and chalcogen analogues

P-66.5.0 Introduction

Compounds with the general structure $R\text{-}C{\equiv}N$ are called ‘nitriles’ or ‘cyanides’. Nitriles and cyanides are derived from hydrocyanic acid, $H\text{-}C{\equiv}N$. When the point of attachment of the $\text{–}C{\equiv}N$ group to ‘R’ is a carbon atom or a heteroatom, these compounds form the class of nitriles and are named substitutively as nitriles. They may also be named as cyanides according to the principles of functional class nomenclature. In substitutive nomenclature formonitrile is the preferred IUPAC name. So, when substituted the compound is a preferred IUPAC name.

These two types of nomenclature are fully discussed in this Section.

P-66.5.1 Nomenclature for generating preferred names of nitriles

Compounds of the general structure $R\text{-}C{\equiv}N$ have the class names ‘nitriles’ and are named in three ways:

(1) substitutively, using the suffixes ‘nitrile’ for –(C)N and ‘carbonitrile for –CN;

(2) by changing the ‘ic acid’ or ‘oic acid’ endings in retained names of carboxylic acids into ‘onitrile’; the nomenclatural properties of acids are transferred to nitriles; thus, preferred names of nitriles correspond to preferred names of carboxylic acids (see P-65.1.1.1) and carboxylic acids that are not substitutable generate nonsubstitutable nitriles (see P-65.1.1.2)

(3) by functional class nomenclature, using the class name ‘cyanide’

P-66.5.1.1 Substitutive and functional class names for nitriles

P-66.5.1.1.1 Acyclic mono- and dinitriles are named in the following two ways:

(1) substitutively by using the suffix ‘nitrile’; and

(2) by functional class nomenclature using the class name ‘cyanide’.

Method (1) leads to preferred IUPAC names.

Examples:

$$\overset{6}{C}H_3\text{-}[CH_2]_4\text{-}\overset{1}{C}N$$

hexanenitrile (PIN)
pentyl cyanide

$$N\overset{5}{C}\text{-}\overset{4}{C}H_2\text{-}\overset{3}{C}H_2\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}N$$

pentanedinitrile (PIN)
propane-1,3-diyl dicyanide

P-66.5.1.1.2 If an unbranched alkane is linked to more than two terminal cyano groups, all cyano groups are named from the parent hydride by the substitutive suffix ‘carbonitrile’, preceded by appropriate multiplying prefix and locants.

Example:

$$\overset{4}{C}H_3\text{-}[CH_2]_2\text{-}\overset{1}{C}(CN)_3$$

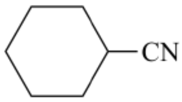
butane-1,1,1-tricarbonitrile (PIN)

P-66.5.1.1.3 The suffix ‘carbonitrile’ is always used to name nitriles having the –CN group attached to a ring or ring system or to an acyclic heteroatom.

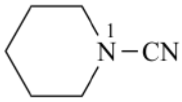
Examples:

$H_3Si\text{-}CN$
silanecarbonitrile (PIN)
silyl cyanide

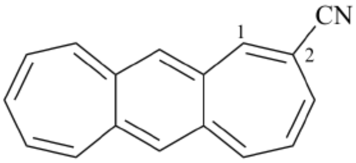
$H_2N\text{-}NH\text{-}CN$
hydrazinecarbonitrile
cyanohydrazide (PIN; see P-66.3.1.2.1)
hydrazinyl cyanide (see P-66.5.1.3)



cyclohexanecarbonitrile (PIN)
cyclohexyl cyanide



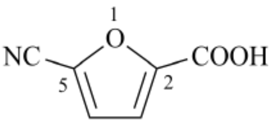
piperidine-1-carbonitrile (PIN)



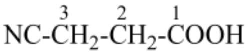
(benzo[1,2:4,5]di[7]annulene)-2-carbonitrile (PIN)
(benzo[1,2:4,5]dicycloheptene)-2-carbonitrile

P-66.5.1.1.4 When a group is present that has priority for citation as the principal characteristic group or when all –CN groups cannot be expressed as the principal characteristic group, the –CN group is designated by the preferred prefix ‘cyano’. The prefix ‘cyano’ must also be used when the –CN group is located at the end of a chain.

Examples:

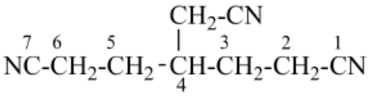


5-cyanofuran-2-carboxylic acid (PIN)
5-cyano-2-furoic acid



$$\text{NC-}\overset{3}{\text{C}}\text{H}_2\text{-}\overset{2}{\text{C}}\text{H}_2\text{-}\overset{1}{\text{C}}\text{OOH}$$

3-cyanopropanoic acid (PIN)



$$\overset{7}{\text{N}}\overset{6}{\text{C}}\text{-CH}_2\text{-}\overset{5}{\text{C}}\text{H}_2\text{-}\underset{4}{\overset{\overset{\text{CH}_2\text{-CN}}{|}}{\text{C}}}\text{H-}\overset{3}{\text{C}}\text{H}_2\text{-}\overset{2}{\text{C}}\text{H}_2\text{-}\overset{1}{\text{C}}\text{N}$$

4-(cyanomethyl)heptanedinitrile (PIN)

P-66.5.1.2 Nitriles derived from retained names of carboxylic acids

P-66.5.1.2.1 The following names are preferred IUPAC names, with unlimited substitution, except for formonitrile whose substitution rules are the same as formic acid (see P-65.1.8) and, obviously, for oxalonitrile for which no substitution is possible.

HCN
formonitrile(PIN)
methanenitrile
hydrogen cyanide

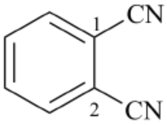
CH_3-CN
acetonitrile (PIN)
ethanenitrile

C_6H_5-CN
benzonitrile (PIN)
benzenecarbonitrile

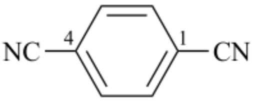
NC-CN
oxalonitrile (PIN)
ethanedinitrile

P-66.5.1.2.2 For general nomenclature, only the names furonitrile, phthalonitrile, isophthalonitrile, and terephthalonitrile are retained with full substitution allowed (see P-65.1.1.2.1). Systematic names (see P-65.1.2) are the preferred IUPAC names.

Examples:



phthalonitrile
benzene-1,2-dicarbonitrile (PIN)



terephthalonitrile
benzene-1,4-dicarbonitrile (PIN)

P-66.5.1.2.3 Nitriles derived from retained acid names given in P-65.1.1.2.2 are only used in general nomenclature; no substitution is allowed. Preferred IUPAC names are systematic names (see P-66.5.1.1).

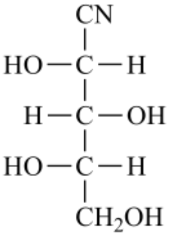
Examples:

CH_3-CH_2-CN
propiononitrile
propanenitrile (PIN)

NC-CH_2-CH_2-CN
succinonitrile
butanedinitrile (PIN)

P-66.5.1.2.4 Names of nitriles derived from carbohydrate acids and amino acids are discussed in P-102.5.6.6.2.1 and P-103.2.8, respectively.

Examples:



L-xylononitrile (see P-102.5.6.6.2.1)

H_2N-CH_2-CN
aminoacetonitrile (see P-103.2.8)
glycinonitrile

P-66.5.1.3 Functional class nomenclature for generating preferred IUPAC names of cyanides

Functional class nomenclature is used, when needed, to name compounds in accordance with the seniority of classes and to name compounds that cannot be named substitutively, for example, cyanides corresponding to sulfonic acid, sulfinic acids and their selenium and tellurium analogues, carbonic acid, cyanic acid, and inorganic acids.

P-66.5.1.3.1 Nitriles with an α-oxo group.

Compounds of the type R-CO-CN can be named as acyl cyanides in a way similar to acid halides. Since acyl cyanides are senior to nitriles, in the seniority of classes, functional class nomenclature must be used to express correctly the seniority order.

Examples:

HCO-CN
formyl cyanide (PIN)
oxoacetonitrile

CH_3-CO-CN
acetyl cyanide (PIN)
2-oxopropanenitrile

CH_3-$[CH_2]_5$-CO-CN
heptanoyl cyanide (PIN)
2-oxooctanenitrile

NC-CO-CO-CN
oxalyl dicyanide (PIN)
2,3-dioxobutanedinitrile

P-66.5.1.3.2 Cyanides corresponding to the sulfur, selenium, and tellurium acids Cyanides formally formed by replacing the –OH group of sulfonic acids, sulfinic acids, and similar Se and Te acids are named by functional class nomenclature.

Examples:

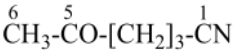
CH_3-SO_2-CN
methanesulfonyl cyanide (PIN)

C_6H_5-SeO-CN
benzeneseleninyl cyanide (PIN)

P-66.5.2 Substituted nitriles

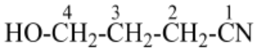
Substituents on the parent hydrides are denoted as prefixes. Nitriles, in the seniority order of classes, are senior to ketones, pseudoketones, heterones, hydroxy compounds, amines, and imines; these classes must be cited as prefixes in the presence of a nitrile group. Seniority for numbering of polyfunctional nitriles follows that described for acids, for which see P-65.1.2.3 and P-65.1.2.4.

Examples:



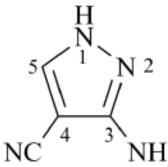
$\overset{6}{C}H_3\text{-}\overset{5}{C}O\text{-}[CH_2]_3\text{-}\overset{1}{C}N$

5-oxohexanenitrile (PIN)

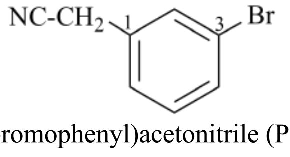


$HO\text{-}\overset{4}{C}H_2\text{-}\overset{3}{C}H_2\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}N$

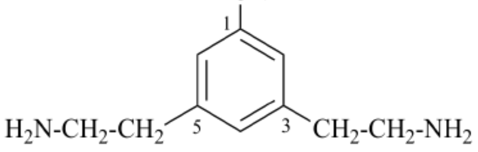
4-hydroxybutanenitrile (PIN)
(not 4-hydroxybutyronitrile;
no substitution for this retained name, see P-65.1.1.2)



3-amino-1*H*-pyrazole-4-carbonitrile (PIN)

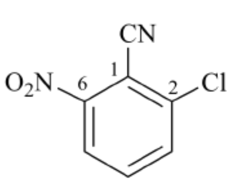


(3-bromophenyl)acetonitrile (PIN)

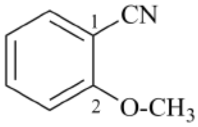


3,5-bis(2-aminoethyl)benzonitrile (PIN)

NC-CH_2-CH_2-NH-CH_2-CH_2-CN
3,3′-azanediyldipropanenitrile (PIN)
(not 3,3′-azanediyldipropionitrile;
no substitution on propionitrile, see P-65.1.1.2)



2-chloro-6-nitrobenzonitrile (PIN)



2-methoxybenzonitrile (PIN)

$\mathrm{Cl\text{-}\overset{3}{C}H_2\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}O\text{-}CN}$

3-chloropropanoyl cyanide (PIN)
4-chloro-2-oxobutanenitrile
(not 3-chloropropionyl cyanide)

P-66.5.3 Nitriles/cyanides corresponding to carbonic, and di- and polycarbonic acids

P-66.5.3.1 Nitriles corresponding to carbonic acid and di- and polycarbonic acids are named by functional class nomenclature.

Examples:

NC-CO-CN
carbonyl dicyanide (PIN)
2-oxopropanedinitrile
(not oxomalononitrile;
no substitution allowed on malononitrile)

NC-CO-CO-CN
oxalyl dicyanide (PIN)
2,3-dioxobutanedinitrile

NC-C(=NH)-CN
carbonimidoyl dicyanide (PIN)
(not 2-iminopropanedinitrile)

$\mathrm{NC\text{-}C(=NNH_2)\text{-}CN}$
carbonohydrazonoyl dicyanide (PIN)
(not 2-hydrazonopropanedinitrile)

$\mathrm{H_2N\text{-}CO\text{-}CN}$
carbamoyl cyanide (PIN)

NC-CO-O-CO-CN
dicarbonic dicyanide (PIN) (see P-65.5.3.2)

P-66.5.4 Nitrile oxides and chalcogen analogues

P-66.5.4.1 Compounds with the general structure R-C≡NO have the generic name 'nitrile oxides'. As they may be considered as zwitterions, they are classed with zwitterions in the order of compound classes. They are named by three methods:

(1) by the term 'oxide', 'sulfide', 'selenide', or 'telluride' added to the name of the nitrile (see P-74.2.2.2.1.2).

(2) by applying the λ-convention and oxo substitution to the nitrogen atom (see P-14.1);

(3) as zwitterions (see P-74.2.2.2.1.2).

Method (1) leads to preferred IUPAC names

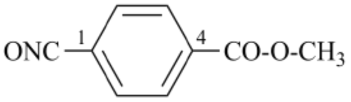
Examples:

$\mathrm{C_6H_5\text{-}C{\equiv}N^+\text{–}O^-}$
(1) benzonitrile oxide (PIN)
(2) benzylidyne(oxo)-λ^5-azane
(3) (benzylidyneazaniumyl)oxidanide

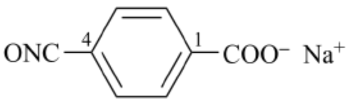
$\mathrm{HC{\equiv}N^+\text{–}O^-}$
(1) formonitrile oxide (PIN)
(2) methylidyne(oxo)-λ^5-azane
(3) (methylidyneazaniumyl)oxidanide

P-66.5.4.2 When it is necessary to cite the group –C≡NO as a substituent prefix, method (2), above is applied.

Examples:



4-(methoxycarbonyl)benzonitrile oxide (PIN)
(not methyl 4-[(oxo-λ^5-azanylidyne)methyl]benzoate)
(no longer methyl 4-isofulminatobenzoate)



sodium 4-[(oxo-λ^5-azanylidyne)methyl]benzoate (PIN)
(no longer sodium 4-isofulminatobenzoate)

P-66.6 ALDEHYDES

P-66.6.0 Introduction
P-66.6.1 Systematic names of aldehydes
P-66.6.2 Aldehydes from di- and polycarbonic acids
P-66.6.3 Chalcogen analogues of aldehydes
P-66.6.4 Polyfunctional aldehydes
P-66.6.5 Acetals and ketals, hemiacetals and hemiketals, and their chalcogen analogues

P-66.6.0 Introduction.

The class name ‘aldehyde’ traditionally refers to compounds containing the –CH=O group attached to a carbon atom. However, nomenclature for aldehydes has been extended to describe a –CHO group attached to a heteroatom.

P-66.6.1 Systematic names of aldehydes

Aldehydes are systematically named in three ways:

(1) substitutively, using the suffixes ‘al’ for –(C)HO and ‘carbaldehyde’ for –CHO;

(2) by changing the ‘ic acid’ or ‘oic acid’ endings of retained names of carboxylic acids into ‘aldehyde’; the nomenclatural properties of acids are transferred to aldehydes; thus, preferred names of aldehydes correspond to preferred names of acids, and carboxylic acids that are not substitutable generate nonsubstitutable aldehydes;

(3) by using the prefixes ‘oxo’, denoting =O, or ‘formyl-’, denoting the substituent group –CHO.

P-66.6.1.1 Names based on suffixes

P-66.6.1.1.1 Mono- and dialdehydes derived from alkanes are named substitutively using the suffix ‘al’ added to the name of the parent hydride with elision of the final letter ‘e’ of the parent hydride before ‘a’.

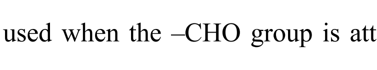
Examples:

CH_3-CH_2-CH_2-CH_2-CHO
pentanal (PIN)

OHC-CH_2-CH_2-CH_2-CHO
pentanedial (PIN)

P-66.6.1.1.2 The suffix ‘carbaldehyde’ is used when more than two –CHO groups are attached to an unbranched alkane chain.

Example:

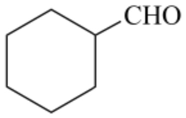


$$\mathrm{OHC\text{-}\overset{1}{C}H_2\text{-}\underset{2}{\overset{CHO}{\overset{|}{C}}}H\text{-}\overset{3}{C}H_2\text{-}\overset{4}{C}H_2\text{-}CHO}$$

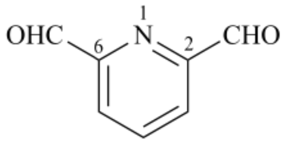
butane-1,2,4-tricarbaldehyde (PIN)

P-66.6.1.1.3 The suffix ‘carbaldehyde’ is used when the –CHO group is attached to a carbon atom of a ring or ring system, or to a heteroatom.

Examples:



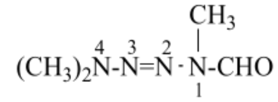
cyclohexanecarbaldehyde (PIN)



pyridine-2,6-dicarbaldehyde (PIN)

$H_2P\text{-}CHO$
phosphanecarbaldehyde (PIN)

$H_2NNH\text{-}CHO$
hydrazinecarbaldehyde
formohydrazide (PIN;
hydrazide is senior to an aldehyde)



$$(\mathrm{CH_3})_2\overset{4}{\mathrm{N}}\text{-}\overset{3}{\mathrm{N}}{=}\overset{2}{\mathrm{N}}\cdot\underset{1}{\overset{\mathrm{CH_3}}{\mathrm{N}}}\text{-}\mathrm{CHO}$$

1,4,4-trimethyltetraaz-2-ene-1-carbaldehyde (PIN)

P-66.6.1.2 Names of aldehydes derived from retained names of carboxylic acids

Names of aldehydes derived from retained names are formed by changing the ‘ic acid’ or ‘oic acid’ ending of the retained names of carboxylic acids to ‘aldehyde’. Substitution of aldehydes parallels that of corresponding carboxylic acids (see P-65.1.1.2).

P-66.6.1.2.1 The following names are preferred IUPAC names, with substitution allowed for acetaldehyde and benzaldehyde. Substitution rules for formaldehyde are the same as for formic acid (see P-65.1.8).

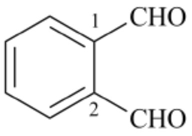
HCHO
formaldehyde (PIN)
methanal

$CH_3\text{-}CHO$
acetaldehyde (PIN)
ethanal

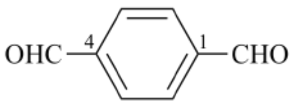
$C_6H_5\text{-}CHO$
benzaldehyde (PIN)
benzenecarbaldehyde

P-66.6.1.2.2 For general nomenclature, only the names furaldehyde, phthalaldehyde, isophthalaldehyde, and terephthalaldehyde are retained with substitution allowed (see P-34). Systematic names (P-66.6.1.1) are the preferred IUPAC names.

Examples:



phthalaldehyde
benzene-1,2-dicarbaldehyde (PIN)



terephthalaldehyde
benzene-1,4-dicarbaldehyde (PIN)

P-66.6.1.2.3 Aldehydes derived from retained acid names given in P-65.1.1.2 are only used in general nomenclature; no substitution is allowed. Preferred IUPAC names are systematic names (see P-66.6.1.1)

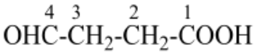
Examples:

$CH_3\text{-}CH_2\text{-}CHO$
propionaldehyde
propanal (PIN)

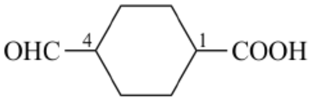
$OHC\text{-}CH_2\text{-}CH_2\text{-}CHO$
succinaldehyde
butanedial (PIN)

P-66.6.1.3 In the presence of a characteristic group having priority to be cited as a suffix or when present on a side chain, a –CHO group is expressed by the preferred prefix ‘oxo’ if located at an end of a carbon chain, or, otherwise, by the preferred prefix ‘formyl’.

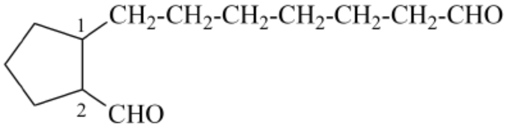
Examples:


$\overset{4\ 3}{OHC}\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}H_2\text{-}COOH$

4-oxobutanoic acid (PIN)
3-formylpropanoic acid



4-formylcyclohexane-1-carboxylic acid (PIN)



2-(7-oxoheptyl)cyclopentane-1-carbaldehyde (PIN)
7-(2-formylcyclopentyl)heptanal
(ring preferred to chain: see P-44.1.2.2)

P-66.6.2 Aldehydes from di- and polycarbonic acids

Aldehydes from di- and polycarbonic acids are named on the basis of the higher compound class. Multiplicative names based on formaldehyde can be used (see P-15.3.2.1).

Examples:

O=CH-O-CH=O
formic anhydride (PIN)
(anhydride senior to aldehyde; see P-41)

O=CH-O-CO-O-CH=O
carbonic diformic dianhydride (PIN)
(anhydride senior to ester; see P-41)
bis(oxomethyl) carbonate

P-66.6.3 Chalcogen analogues of aldehydes

Chalcogen analogues of aldehydes are named by using the suffixes and prefixes in Table 6.4. In the seniority order of classes, aldehydes are senior to ketones, hydroxy compounds, amines, and imines. Names of chalcogen analogues corresponding to aldehydes with retained names are all systematically formed.

Table 6.4 Suffixes and prefixes for chalcogen analogues of aldehydes

Group	Suffix	Prefix
–(C)HS	thial	sulfanylidene (preferred prefix) thioxo
–(C)HSe	selenal	selanylidene (preferred prefix) selenoxo
–(C)HTe	tellanal	tellanylidene (preferred prefix) telluroxo
–CHS	carbothialdehyde	methanethioyl (preferred prefix) thioformyl
–CHSe	carboselenaldehyde	methaneselenoyl (preferred prefix) selenoformyl
–CHTe	carbotelluraldehyde	methanetelluroyl (preferred prefix) telluroformyl

Examples:

$\overset{2}{C}H_3\text{-}\overset{1}{C}HS$

ethanethial (PIN)
thioacetaldehyde

$C_6H_5\text{-}CHS$

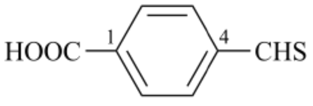
benzenecarbothialdehyde (PIN)
thiobenzaldehyde

$\overset{6}{C}H_3\text{-}[CH_2]_4\text{-}\overset{1}{C}HSe$

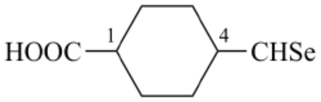
hexaneselenal (PIN)

$SH\overset{5}{C}\text{-}\overset{4}{C}H_2\text{-}\overset{3}{C}H_2\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}HS$

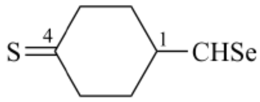
pentanedithial (PIN)



4-(methanethioyl)benzoic acid (PIN)
4-(thioformyl)benzoic acid



4-(methaneselenoyl)cyclohexane-1-carboxylic acid (PIN)
4-(selenoformyl)cyclohexane-1-carboxylic acid



4-sulfanylidenecyclohexane-1-carboselenaldehyde (PIN)
4-thioxocyclohexane-1-carboselenaldehyde

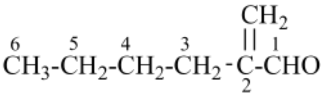
P-66.6.4 Polyfunctional aldehydes

In the presence of an aldehyde group, ketones, pseudoketones, heterones, hydroxy compounds, amines, and imines are expressed by prefixes. Seniority for numbering polyfunctional aldehydes follows that described for acids, for which see P-65.1.2.3 and P-65.1.2.4.

Examples:

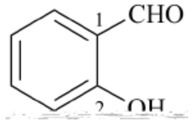
$\overset{4}{C}H_3\text{-}\overset{3}{C}O\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}HO$

3-oxobutanal (PIN)
(not 3-oxobutyraldehyde)

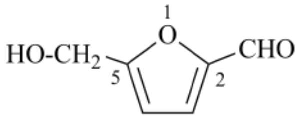


$\overset{6}{C}H_3\text{-}\overset{5}{C}H_2\text{-}\overset{4}{C}H_2\text{-}\overset{3}{C}H_2\text{-}\underset{2}{\overset{\overset{CH_2}{||}}{C}}\text{-}\overset{1}{C}HO$

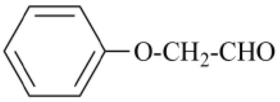
2-methylidenehexanal (PIN)
[not 2-butylprop-2-enal,
the longest chain is the principal chain (see P-44.3)]



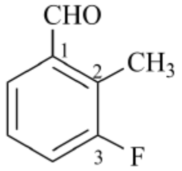
2-hydroxybenzaldehyde (PIN)
(not salicylaldehyde)



5-(hydroxymethyl)furan-2-carbaldehyde (PIN)
5-(hydroxymethyl)-2-furaldehyde
[not 5-(hydroxymethyl)furfural]



phenoxyacetaldehyde (PIN)



3-fluoro-2-methylbenzaldehyde (PIN)

P-66.6.5 Acetals and ketals, hemiacetals and hemiketals, and chalcogen analogues

P-66.6.5.1 Acetals and ketals
P-66.6.5.2 Hemiacetals and hemiketals
P-66.6.5.3 Chalcogen analogues of acetals and ketals

P-66.6.5.1 Acetals and ketals

P-66.6.5.1.1 Compounds with the general structure RR′C(O-R″)(O-R‴), where only R and R′ may be, but need not be, hydrogen, have the class name ‘acetal’. ‘Ketals’ constitute a subclass of acetals wherein neither R nor R′ may be hydrogen. Acetals (ketals) are named in two ways:

(1) substitutively as ‘alkoxy’, alkyloxy, ‘aryloxy’, etc. derivatives of an appropriate parent hydride or functional parent compound;

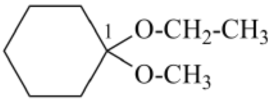
(2) by functional class nomenclature by citing the name of the aldehyde or ketone, the names of the *O*-substituents, in alphanumerical order if required, and finally the class terms ‘acetal’ or ‘ketal’.

Method (1), the substitutive method, leads to preferred IUPAC names.

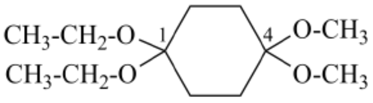
Examples:

$$\overset{3}{C}H_3\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}H(O\text{-}CH_2\text{-}CH_3)_2$$

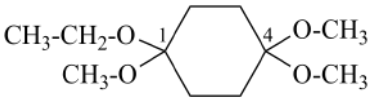
(1) 1,1-diethoxypropane (PIN)
(2) propanal diethyl acetal



(1) 1-ethoxy-1-methoxycyclohexane (PIN)
(2) cyclohexanone ethyl methyl ketal



(1) 1,1-diethoxy-4,4-dimethoxycyclohexane (PIN)
(2) cyclohexane-1,4-dione 1,1-diethyl 4,4-dimethyl diketal



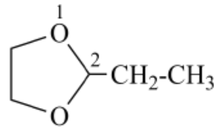
(1) 1-ethoxy-1,4,4-trimethoxycyclohexane (PIN)
(2) cyclohexane-1,4-dione 1-ethyl 1,4,4-trimethyl diketal

P-66.6.5.1.2 Cyclic acetals and ketals

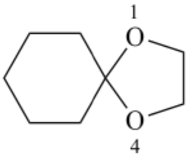
Cyclic acetals as the principal function are named as heterocyclic compounds and these names are preferred IUPAC names; cyclic ketals are spiro compounds that are named in accordance with the rules described in Section P-24 giving preferred IUPAC names.

Functional class nomenclature using the name of the appropriate divalent substituent groups may be used in general nomenclature.

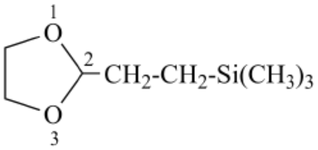
Examples:



2-ethyl-1,3-dioxolane (PIN)
propanal ethylene acetal



1,4-dioxaspiro[4.5]decane (PIN)
cyclohexanone ethylene ketal

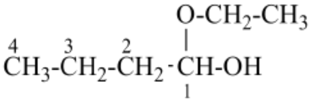


[2-(1,3-dioxolan-2-yl)ethyl]tri(methyl)silane (PIN)
3-(trimethylsilyl)propanal ethylene ketal

P-66.6.5.2 Hemiacetals and hemiketals

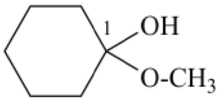
Compounds with the general structure RR′C(OH)(O-R″) have the class name ‘hemiacetals’. They are named substitutively as ‘alkoxy’, ‘alkyloxy’, ‘aryloxy’, etc. derivatives of an appropriate hydroxy parent compound, such as an alcohol; these names are the preferred IUPAC names. Other names are formed by functional class nomenclature using the class name ‘hemiacetal’; similarly derivatives of ketones are denoted by the class name ‘hemiketal’.

Examples:



$$\overset{4}{C}H_3\text{-}\overset{3}{C}H_2\text{-}\overset{2}{C}H_2\text{-}\underset{1}{\overset{O\text{-}CH_2\text{-}CH_3}{\overset{|}{C}}}H\text{-}OH$$

1-ethoxybutan-1-ol (PIN)
butanal ethyl hemiacetal



1-methoxycyclohexan-1-ol (PIN)
cyclohexanone methyl hemiketal

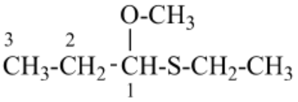
P-66.6.5.3 Chalcogen analogues of acetals and ketals

Sulfur analogues of acetals and ketals with the general structures RR′C(S-R″)(S-R‴), or RR′C(S-R″)(O-R‴), have the class names ‘dithioacetals’ or ‘monothioacetals’, respectively. They are named substitutively as ‘alkylsulfanyl’, ‘arylsulfanyl’, ‘alkoxy’, or ‘aryloxy’ derivatives, as appropriate, of a parent hydride; these names are preferred IUPAC names. Other names can be generated by functional class nomenclature, using class names such as ‘monothioacetal’ and ‘dithioketal’. Capital italic letter locants are used to provide structural specificity. Selenium, tellurium, and mixed chalcogen analogues are treated in the same way as their sulfur analogues.

Examples:

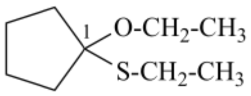
$$\overset{5}{C}H_3\text{-}\overset{4}{C}H_2\text{-}\overset{3}{C}H_2\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}H(S\text{-}CH_3)_2$$

1,1-bis(methylsulfanyl)pentane (PIN)
pentanal dimethyl dithioacetal

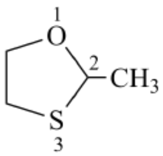


$$\overset{3}{C}H_3\text{-}\overset{2}{C}H_2\text{-}\underset{1}{\overset{O\text{-}CH_3}{\overset{|}{C}}}H\text{-}S\text{-}CH_2\text{-}CH_3$$

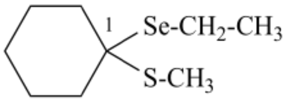
1-(ethylsulfanyl)-1-methoxypropane (PIN)
propanal *S*-ethyl *O*-methyl monothioacetal



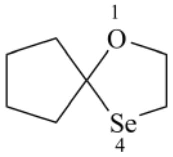
1-ethoxy-1-(ethylsulfanyl)cyclopentane (PIN)
cyclopentanone diethyl monothioketal



2-methyl-1,3-oxathiolane (PIN)
acetaldehyde ethylene monothioacetal



1-(ethylselanyl)-1-(methylsulfanyl)cyclohexane (PIN)
cyclohexanone *Se*-ethyl *S*-methyl selenothioketal

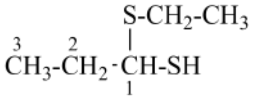


1-oxa-4-selenaspiro[4.4]nonane (PIN)
cyclopentanone ethylene monoselenoketal

P-66.6.5.4 Chalcogen analogues of hemiacetals and hemiketals

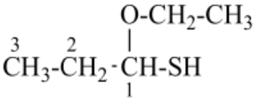
Sulfur analogues of hemiacetals and hemiketals with the general structures RR′C(SH)(S-R″), RR′C(OH)(S-R″) or RR′C(SH)(O-R″), have the class names ‘dithiohemiacetals’ or ‘monothiohemiacetals’, respectively. They are named substitutively as ‘alkylsulfanyl’, ‘arylsulfanyl’, ‘alkoxy’, or ‘aryloxy’ derivatives, as appropriate, of a hydroxy parent compound; these are preferred IUPAC names. Other names can be generated by functional class nomenclature. Capital italic letter locants are used to provide structural specificity. Selenium, tellurium, and mixed analogues are treated in the same way as their sulfur analogues; generically, they are ‘monoselenohemiacetals’, ‘ditellurohemiacetals’, ‘selenothiohemiacetals’, etc.

Examples:



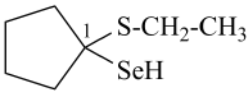
$$\overset{3}{C}H_3\text{-}\overset{2}{C}H_2\text{-}\underset{1}{\overset{\overset{\displaystyle S\text{-}CH_2\text{-}CH_3}{|}}{C}}H\text{-}SH$$

1-(ethylsulfanyl)propane-1-thiol (PIN)
propanal ethyl dithiohemiacetal



$$\overset{3}{C}H_3\text{-}\overset{2}{C}H_2\text{-}\underset{1}{\overset{\overset{\displaystyle O\text{-}CH_2\text{-}CH_3}{|}}{C}}H\text{-}SH$$

1-ethoxypropane-1-thiol (PIN)
propanal *O*-ethyl monothiohemiacetal



1-(ethylsulfanyl)cyclopentane-1-selenol (PIN)
cyclopentanone *S*-ethyl selenothiohemiketal

P-67 MONONUCLEAR AND POLYNUCLEAR NONCARBON ACIDS AND THEIR FUNCTIONAL REPLACEMENT ANALOGUES AS FUNCTIONAL PARENTS FOR NAMING ORGANIC COMPOUNDS

P-67.0 Introduction
P-67.1 Mononuclear noncarbon oxoacids
P-67.2 Di- and polynuclear noncarbon oxoacids
P-67.3 Substitutive names and functional class names of polyacids

P-67.0 INTRODUCTION

Mono-, di-, and polynuclear noncarbon oxoacids and their chalcogen analogues having retained names are used as parent structures to generate names of carbon containing compounds. In these recommendations, the names for these compounds are preselected names (see P-12.2)

Names of chalcogen analogues of noncarbon oxoacids are formed by functional replacement nomenclature. This type of nomenclature is also used to create derived classes, for example, acid halides and pseudohalides, amides, hydrazides, and amidines. With regard to functional replacement, mono- di- and polynuclear noncarbon acids do not constitute a homogeneous group. Names of mononuclear oxoacids are modified by infixes, with the exception of silicic acid, nitrous acid, nitric acid and the halogen acids. Names of the di- and polynuclear noncarbon oxoacids are modified by prefixes. Functional class nomenclature is used to generate names for esters, organic anhydrides, carbon containing pseudohalides such as cyanides and isocyanates, and organic derivatives of amides, imides, and hydrazides.

Mononuclear noncarbon oxoacids are discussed first, then di- and polynuclear noncarbon oxoacids, such as diphosphoric acid, $\mathrm{(HO)_2P(O){-}O{-}P(O)(OH)_2}$, which are named as acids, not as anhydrides, and hypodiphosphoric acid, $\mathrm{(HO)_2P(O){-}P(O)(OH)_2}$.

Systematization has been achieved, taking into consideration the nomenclature of inorganic compounds (ref. 12), that has restricted the use of retained names and of prefixes such as ‘hypo’, ‘ortho’, ‘iso’ added to the names of mononuclear oxoacids to generate retained names. However, the traditional nomenclature of organic compounds derived from mono-, di-, and polynuclear oxoacids has been maintained.

For carbonic, cyanic, di- and polynuclear carbonic acids, see P-65.2.

P-67.1 MONONUCLEAR NONCARBON OXOACIDS

Retained names for mononuclear noncarbon oxoacids have the following elements as central atoms: N, P, As, Sb, Si, B, S, Se, Te, F, Cl, Br, and I. They are used as parent structures and also for derivation of prefixes to be used in the presence of classes that have seniority for being named as parent compounds. These parent structures have retained names that are traditional names used as preselected names (see P-12.2). They may also have systematic additive or substitutive names, but these names are not recommended for generating preselected names (see IR-8, ref. 12)

Functional replacement nomenclature is discussed first; next the formation of esters and anhydrides using functional class nomenclature; and finally, substitutive nomenclature using prefixes is described. Application of the seniority order of oxoacids and their derivatives, described in Section P-42, is discussed. The Section ends with the nomenclature of *aci*-nitro compounds that are named as derivatives of azinic acid.

P-67.1.1 Names for mononuclear noncarbon oxoacids and their derivatives formed by substitution
P-67.1.2 Functional replacement nomenclature applied to noncarbon oxoacids
P-67.1.3 Salts, esters, and anhydrides of noncarbon oxoacids
P-67.1.4 Substituent prefix groups derived from mononuclear noncarbon oxoacids
P-67.1.5 Seniority order among noncarbon oxoacids and derivatives
P-67.1.6 *aci*-Nitro compounds

P-67.1.1 Names for mononuclear noncarbon oxoacids and their derivatives formed by substitution

P-67.1.1.1 Names of mononuclear noncarbon oxoacids

Preselected names (see P-12.2) of the mononuclear noncarbon oxoacids used for deriving preferred IUPAC names for organic compounds and names for general organic nomenclature are noted in the following list, given in alphabetical order.

$\mathrm{H_2As(O)(OH)}$	arsinic acid (preselected name)
$\mathrm{H_2As(OH)}$	arsinous acid (preselected name)
$\mathrm{HAs(O)(OH)_2}$	arsonic acid (preselected name)
$\mathrm{HAs(OH)_2}$	arsonous acid (preselected name)
$\mathrm{As(O)(OH)_3}$	arsoric acid (preselected name) arsenic acid

Note: Arsoric acid is preferred to arsenic acid as the preselected name for clarity and consistency with phosphoric acid.

$\mathrm{As(OH)_3}$	arsorous acid (preselected name) (formerly arsen(i)ous acid)

Note: Arsorous acid is preferred to arsen(i)ous acid as the preselected name for clarity and consistency with phosphorous acid

$\mathrm{H_2N(O)(OH)}$	azinic acid (preselected name)
$\mathrm{H_2N{-}OH}$	azinous acid hydroxylamine (preselected name, for which see P-68.3.1.1.1)
$\mathrm{HN(O)(OH)_2}$	azonic acid (preselected name)

$HN(OH)_2$	azonous acid (preselected name)
$N(O)(OH)_3$	nitroric acid (preselected name)
$N(OH)_3$	azorous acid (preselected name)
$B(OH)_3$	boric acid (preselected name)
$H_2B(OH)$	borinic acid (preselected name)
$HB(OH)_2$	boronic acid (preselected name)
$Br(O)_2(OH)$	bromic acid (preselected name)
$Br(O)(OH)$	bromous acid (preselected name)
$Cl(O))_2(OH)$	chloric acid (preselected name)
$Cl(O)(OH)$	chlorous acid (preselected name)
$Br(OH)$	hypobromous acid (preselected name)
$Cl(OH)$	hypochlorous acid (preselected name)
$F(OH)$	hypofluorous acid (preselected name)
$I(OH)$	hypoiodous acid (preselected name)
$I(O)_2(OH)$	iodic acid (preselected name)
$I(O)(OH)$	iodous acid (preselected name)
$HO\text{-}NO_2$	nitric acid (preselected name)
$HO\text{-}NO$	nitrous acid (preselected name)
$Br(O)_3(OH)$	perbromic acid (preselected name)
$Cl(O)_3(OH)$	perchloric acid (preselected name)
$F(O)_3(OH)$	perfluoric acid (preselected name)
$I(O)_3(OH)$	periodic acid (preselected name)
$H_2P(O)(OH)$	phosphinic acid (preselected name)
$H_2P(OH)$	phosphinous acid (preselected name)
$HP(O)(OH)_2$	phosphonic acid (preselected name)
$HP(OH)_2$	phosphonous acid (preselected name)
$P(O)(OH)_3$	phosphoric acid (preselected name)
$P(OH)_3$	phosphorous acid (preselected name)
$Se(O)_2(OH)_2$	selenic acid (preselected name)
$Se(O)(OH)_2$	selenous acid (preselected name)
$Si(OH)_4$	silicic acid (preselected name) (not orthosilicic acid)
$H_2Sb(O)(OH)$	stibinic acid (preselected name)
$H_2Sb(OH)$	stibinous acid (preselected name)
$HSb(O)(OH)_2$	stibonic acid (preselected name)
$HSb(OH)_2$	stibonous acid (preselected name)
$Sb(O)(OH)_3$	stiboric acid (preselected name) antimonic acid

Note: Stiboric acid is preferred to antimonic acid as the preselected name for clarity and consistency with stibonic and with phosphoric and arsoric acid

$Sb(OH)_3$	stiborous acid (preselected name) antimonous acid

Note: Stiborous acid is preferred to antimonous acid as the preselected name for clarity and consistency with stibonic acid and with phosphorous and arsorous acid

$S(O)_2(OH)_2$	sulfuric acid (preselected name)
$S(O)(OH)_2$	sulfurous acid (preselected name)
$Te(O)_2(OH)_2$	telluric acid (preselected name)
$Te(O)(OH)_2$	tellurous acid (preselected name)

P-67.1.1.2 Substitution of mononuclear noncarbon oxoacids with hydrogen atoms attached to the central atom (substitutable hydrogen)

Acids with hydrogen atoms attached to the central atom may be substituted by organyl groups and preferred IUPAC names are formed in this manner.

Note: Another method has been suggested which would treat the acid as a suffix (like sulfonic acid) leading to names such as benzenephosphonic acid. This suggestion has been rejected because in cases where the acid has two substitutable hydrogen atoms, the use of additional letter locants would be required leading to unnecessarily more cumbersome names.

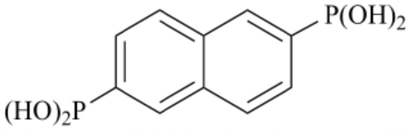
Examples:

$C_2H_5\text{-}P(O)(OH)_2$
ethylphosphonic acid (PIN)
(not ethanephosphonic acid)

$(C_2H_5)_2P(O)(OH)$
diethylphosphinic acid (PIN)
(not *P*-ethylethanephosphinic acid)

$(C_6H_5)_2As(OH)$
diphenylarsinous acid (PIN)

$C_6H_5Sb(OH)_2$
phenylstibonous acid (PIN)



(naphthalene-2,6-diyl)bis(phosphonous acid) (PIN)

P-67.1.2 Functional replacement nomenclature applied to mononuclear noncarbon oxoacids

Mononuclear noncarbon oxoacids are modified by either infixes or prefixes in functional replacement nomenclature.

P-67.1.2.1 Mononuclear acids modified by infixes
P-67.1.2.2 Mononuclear acids modified by prefixes
P-67.1.2.3 General methodology for functional replacement nomenclature using infixes
P-67.1.2.4 Mononuclear noncarbon oxoacids modified by functional replacement nomenclature
P-67.1.2.5 Acid halides and pseudohalides
P-67.1.2.6 Amides and hydrazides

P-67.1.2.1 Mononuclear noncarbon oxoacids modified by infixes. The following acids are modified by infixes; they are listed in group order B, N, P, As, Sb, S, Se, Te:

$B(OH)_3$	boric acid
$HB(OH)_2$	boronic acid
$H_2B(OH)$	borinic acid
$N(O)(OH)_3$	nitroric acid (hypothetical)
$N(OH)_3$	azorous acid (hypothetical)
$HN(O)(OH)_2$	azonic acid
$H_2N(O)(OH)$	azinic acid
$HN(OH)_2$	azonous acid
$P(O)(OH)_3$	phosphoric acid
$P(OH)_3$	phosphorous acid
$HP(O)(OH)_2$	phosphonic acid
$HP(OH)_2$	phosphonous acid
$H_2P(O)(OH)$	phosphinic acid
$H_2P(OH)$	phosphinous acid
$As(O)(OH)_3$	arsoric acid (formerly arsenic acid)
$As(OH)_3$	arsorous acid (formerly arsen(i)ous acid)
$HAs(O)(OH)_2$	arsonic acid
$HAs(OH)_2$	arsonous acid
$H_2As(O)(OH)$	arsinic acid
$H_2As(OH)$	arsinous acid
$Sb(O)(OH)_3$	stiboric acid (formerly antimonic acid)
$Sb(OH)_3$	stiborous acid (formerly antimonous acid)
$HSb(O)(OH)_2$	stibonic acid

$HSb(OH)_2$	stibonous acid
$H_2Sb(O)(OH)$	stibinic acid
$H_2Sb(OH)$	stibinous acid
$S(O)_2(OH)_2$	sulfuric acid
$S(O)(OH)_2$	sulfurous acid
$Se(O)_2(OH)_2$	selenic acid
$Se(O)(OH)_2$	selenous acid
$Te(O)_2(OH)_2$	telluric acid
$Te(O)(OH)_2$	tellurous acid

P-67.1.2.2 Mononuclear noncarbon oxoacids modified by prefixes. The following acids are modified by prefixes; they are listed in the order Si, N, F, Cl, Br, I.

$Si(OH)_4$	silicic acid (formerly orthosilicic acid)
$HO\text{-}NO_2$	nitric acid
HO-NO	nitrous acid
$F(O)_3(OH)$	perfluoric acid
$F(O)_2(OH)$	fluoric acid
F(O)(OH)	fluorous acid
F(OH)	hypofluorous acid
$Cl(O)_3(OH)$	perchloric acid
$Cl(O)_2(OH)$	chloric acid
Cl(O)(OH)	chlorous acid
Cl(OH)	hypochlorous acid
$Br(O)_3(OH)$	perbromic acid
$Br(O)_2(OH)$	bromic acid
Br(O)(OH)	bromous acid
Br(OH)	hypobromous acid
$I(O)_3(OH)$	periodic acid
$I(O)_2(OH)$	iodic acid
I(O)(OH)	iodous acid
I(OH)	hypoiodous acid

P-67.1.2.3 General methodology for functional replacement nomenclature using infixes

Functional replacement nomenclature (see P-15.5) using infixes generates functional class names for the following classes: acid halides and pseudo halides (azides, cyanides, isocyanides, and isocyanates), amides, hydrazides, and also imidic, hydrazonic and nitridic acids. Chalcogen analogues are also described by infixes.

Note: Preferred IUPAC names are retained names modified by functional nomenclature. The use of infixes is restricted to acids listed in P-67.1.2.1 and leads to preferred IUPAC names. Prefixes are used as recommended for acids listed in P-67.1.2.2, and in general nomenclature for all mononuclear acids. Substitutive names and names modified by prefixes are used only in special occasions (see P-67.1.4.1.1.6 and P-67.3.1).

Example:

$(C_6H_5)_2P\text{-}SH$
diphenylphosphinothious acid (PIN)
(not diphenylphosphanethiol)
[not diphenyl(sulfanyl)phosphane]

P-67.1.2.3.1 The following infixes are used to describe the replacement of =O and –OH by chalcogen analogues (in decreasing order of seniority):

(1)	–OO–	peroxo
(2)	–OS– or –SO–	thioperoxo (similarly selenoperoxo, telluroperoxo)
(3)	–SS–	dithioperoxo (similarly diselenoperoxo, ditelluroperoxo)

(4)	–SSe– or –SeS–	selenothioperoxo (similarly for other mixed chalcogens)
(5)	–S– or =S	thio
(6)	–Se– or =Se	seleno
(7)	–Te– or =Te	telluro

P-67.1.2.3.2 Infixes denoting replacement of -OH group in decreasing order of seniority with all halides (class 1) and pseudohalides (class 2) having the same rank within the class.

(1)	–Br	bromido
	–Cl	chlorido
	–F	fluorido
	–I	iodido
(2)	$–N_3$	azido
	–OCN	cyanatido
	–CN	cyanido
	–NCO	isocyanatido
	–NC	isocyanido
	–NCSe	isoselenocyanatido
	–NCTe	isotellurocyanatido
	–NCS	isothiocyanatido
	–SeCN	selenocyanatido
	–TeCN	tellurocyanatido
	–SCN	thiocyanatidoo
(3)	$–NH_2$	amido
(4)	$–NH\text{-}NH_2$	hydrazido
(5)	≡N	nitrido
(6)	=NH	imido
(7)	$=NNH_2$	hydrazono

P-67.1.2.3.3 Prefixes denoting chalcogen analogues of acids by replacing oxygen atoms (in decreasing order of seniority):

(1)	–OO–	peroxo
(2)	–OS– or –SO–	thioperoxy (similarly selenoperoxy, telluroperoxy)
(3)	–SS–	dithioperoxy (similarly diselenoperoxy, ditelluroperoxy)
(4)	–SSe– or –SeS–	selenothioperoxy (similarly for other mixed chalcogens)
(5)	–S– or =S	thio
(6)	–Se– or =Se	seleno
(7)	–Te– or =Te	telluro

P-67.1.2.3.4 Prefixes denoting replacement of -OH group in decreasing order of seniority with all halides (class 1) and pseudohalides (class 2) having the same rank within the class.

(1)	–Br	bromo
	–Cl	chloro
	–F	fluoro
	–I	iodo
(2)	$–N_3$	azido
	–OCN	cyanato
	–CN	cyano
	–NCO	isocyanato
	–NC	isocyano
	–NCSe	isoselenocyanato

	–NCTe	isotellurocyanato
	–NCS	isothiocyanato
	–SeCN	selenocyanato
	–TeCN	tellurocyanato
	–SCN	thiocyanato
(4)	$–NH\text{-}NH_2$	hydrazido
(5)	≡N	nitrido
(6)	=NH	imido
(7)	$=NNH_2$	hydrazono

P-67.1.2.3.5 The appropriate infix is indicated (in alphabetical order if more than one) before the ‘ic acid’ or ‘ous acid’ ending in the parent name, with elision of the letter ‘o’ before a vowel, with the exception of the infixes ‘thio’, ‘seleno’, ‘telluro’ and ‘peroxo’ which are cited as such, with no elision of the letter ‘o’, before the ‘ic ending’. An euphonic letter ‘o’ also may be added when necessary. Multiplying an infix by multiplying prefixes ‘di’ or ‘tri’ does not change its place in the alphabetical order.

The appropriate prefix is indicated (in alphabetical order if there is more than one) before the name of the acid; no elision is recommended. Multiplying a prefix by multiplying prefixes ‘di’ or ‘tri’ does not change its place in the alphabetical order.

P-67.1.2.4 Mononuclear noncarbon oxoacids modified by functional replacement nomenclature

Preselected names described in P-67.1.2 are used for deriving preferred IUPAC names for organic compounds. As long as there is at least one –OH group left in an oxoacid having a retained name, the acid modified by functional replacement is classified as an acid and denoted by class name ‘acid’.

P-67.1.2.4.1 Functional replacement of the oxoacids specifically listed in P-67.1.2 is expressed by infixes or prefixes. Substitution of nonacidic hydrogen atoms is indicated by prefixes, with a letter locant B, N, P, As or Sb, as needed. Tautomers may be distinguished by prefixing italic elements symbols, such as S and O, to the term ‘acid’. Parentheses are needed to enclose infixes modified by a chalcogen prefix, for example, ‘thioperoxoic’. In addition to infixes and prefixes listed in P-67.1.2.3, the prefix ‘cyanato’ and the infix ‘cyanatido’, for –OCN, are used to modify acids as indicated in P-67.1.2.4.1.3.

P-67.1.2.4.1.1 Examples of mononuclear noncarbon oxoacids modified by infixes:

$CH_3\text{-}B(OH)(SH)$
methylboronothioic acid (PIN)

$CH_3\text{-}B(NH\text{-}CH_3)(OH)$
B,*N*-dimethylboronamidic acid (PIN)

$CH_3\text{-}N(OH)(SH)$
methylazonothious acid (PIN)

$(C_2H_5)_2P(S)(SH)$
diethylphosphinodithioic acid (PIN)

$(CH_3)_2N\text{-}P(O)(OH)_2$
dimethylphosphoramidic acid (PIN)

$(C_6H_5)_2P(=N\text{-}CH_3)(OH)$
N-methyl-*P*,*P*-diphenylphosphinimidic acid (PIN)

$C_6H_5\text{-}P(=N\text{-}C_6H_5)(Cl)(SH)$
N,*P*-diphenylphosphonochloridimidothioic acid (PIN)

$C_6H_5\text{-}P(S)(NH\text{-}CH_3)(OH)$
N-methyl-*P*-phenylphosphonamidothioic *O*-acid (PIN)

$(CH_3)_2N\text{-}P(O)(NCS)(SH)$
N,*N*-dimethylphosphoramid(isothiocyanatido)thioic *S*-acid (PIN)

$(CH_3)_2N\text{-}P(=N\text{-}C_6H_5)(SCN)(OH)$
N,*N*-dimethyl-*N*′-phenylphosphoramidimido(thiocyanatidic) acid (PIN)

$C_6H_5\text{-}P(OH)(SH)$
phenylphosphonothious acid (PIN)

C_6H_5-P(≡N)(OH)
phenylphosphononitridic acid (PIN)

C_6H_5-P(O)(Cl)(OH)
phenylphosphonochloridic acid (PIN)

CH_3-CH_2-P(Se)$(OH)_2$
ethylphosphonoselenoic *O*,*O*-acid (PIN)

CH_3-CH_2-P(O)(OH)(SeH)
ethylphosphonoselenoic *Se*-acid (PIN)

P(=NH)(NH-NH_2)$(OH)_2$
phosphorohydrazidimidic acid
(name derived from the preselected name phosphoric acid)

P(O)(OH)(SH)(SSH)
phosphoro(dithioperoxo)thioic *S*-acid
(name derived from the preselected name phosphoric acid)

P(O)$(OH)_2$(OSH)
phosphoro(thioperoxoic) *OS*-acid
(name derived from the preselected name phosophoric acid)

As(O)(OH)$(SH)_2$ or As(S)$(OH)_2$(SH)
arsorodithioic acid
(name derived from the preselected name arsoric acid)

As(S)$(OH)_3$
arsorothioic *O*,*O*,*O*-acid
(name derived from the preselected name arsoric acid)

$(C_6H_5)_2$As(SH)
diphenylarsinothious acid (PIN)

HO-SO_2-SH
sulfurothioic *S*-acid
(name derived from the preselected name sulfuric acid)

H_2N-SO_2-OH
sulfamic acid
(name derived from the preselected name sulfuric acid; contraction of sulfuramidic acid)

$H_2S_2O_3$
sulfurothioic acid
(name derived from the preselected name sulfuric acid; the position of the sulfur atom is undetermined)

HO-SO_2-NC
sulfurisocyanidic acid (PIN)

HO-SO_2-NCS
sulfur(isothiocyanatidic) acid (PIN)

HO-SO_2-CN
sulfurocyanidic acid (PIN)

HS-SO_2-NH_2
sulfamothioic *S*-acid
(name derived from the preselected name sulfuric acid; a contraction of sulfuramidothioic *S*-acid)

HS-TeO_2-NH_2
telluramidothioic acid
(name derived from the preselected name telluric acid)

P-67.1.2.4.1.2 Examples of mononuclear noncarbon oxoacids modified by prefixes:

$Si(OH)_3$(SH)
thiosilicic acid
(name derived from the preselected name silicic acid)

S=N-OH
thionitrous *O*-acid
(name derived from the preselected name nitrous acid)

$Cl(S)_2$-OH
dithiochloric *O*-acid
(name derived from the preselected name chloric acid)

P-67.1.2.4.1.3 Specific use of the prefix ‘cyanato’ and the infix ‘cyanatido’

When attached to the central atom of a mononuclear noncarbon oxoacid, the group –OCN creates an anhydride linkage (see P-67.1.3.3). In order to respect the seniority order classes, this group is used, therefore, in functional replacement nomenclature to name acids; acids are senior to anhydrides. For the prefixes ‘cyanato’, ‘thiocyanato’, ‘selenocyanato’ and ‘tellurocyanato’, see P-65.2.2.

Examples:

CH_3-P(O)(OCN)OH
methylphosphonocyanatidic acid (PIN)

$P(O)(OCN)_2OH$
phosphorodicyanatidic acid (PIN)

$Si(OCN)(OH)_3$
cyanatosilicic acid (PIN)

P-67.1.2.4.2 Name construction guidelines for functional replacement nomenclature.

The names phosphonous, phosphinous, phosphonic and phosphinic acid (and similarly for arsenic, antimony and nitrogen acids) can only be used when P, As or Sb is attached to atoms of hydrogen, carbon or another atom of a parent hydride such as N, As, Si. Thus, C_6H_5-P(O)Cl(OH) is phenylphosphonochloridic acid and not chloro(phenyl)phosphinic acid; ($C_5H_{10}N$)-P(O)Cl(OH) is (piperidin-1-yl)phosphonochloridic acid and not chloro(piperidin-1-yl)phosphinic acid; and $ClP(O)(OH)_2$ is phosphorochloridic acid and not chlorophosphonic acid.

P-67.1.2.5 Acid halides and pseudohalides

P-67.1.2.5.1 Except for the boron acids and silicic acid, preferred IUPAC names of acid halides and pseudohalides are formed by adding the class name(s) of a halide or pseudohalide to that of the acid. Exceptionally, in accordance with tradition and the recommended nomenclature of inorganic compounds (ref. 12), halides and pseudohalides with identical atoms or groups and derived from phosphoric acid, sulfuric acid, selenic acid and telluric acid are named by adding the class name(s) to the acyl group name ‘phosphoryl’, ‘sulfuryl’, ‘sulfamoyl’, ‘selenonyl’ and ‘telluronyl’, and not to the name of the acid itself. In accordance with the seniority order of halides and pseudohalides, names are formed on the basis of the senior class, as described in P-67.1.2.1.

Preferred IUPAC names of acid halides and pseudohalides derived from the boron acids and silicic acid are formed on the basis of the parent hydride names borane and silane, respectively.

Examples:

CH_3-$N(O)Cl_2$
methylazonic dichloride (PIN)
$P(O)(NCO)_3$
phosphoryl triisocyanate (PIN)

$(C_6H_5)_2$P-Cl
diphenylphosphinous chloride (PIN)

$(C_6H_5)_2$Sb-NCO
diphenylstibinous isocyanate (PIN)

C_6H_5-PCl_2
phenylphosphonous dichloride (PIN)

C_6H_5-PBrCl
phenylphosphonous bromide chloride (PIN)
phenylphosphonobromidous chloride

$(C_6H_5)_2P(=N-C_6H_5)Cl$
N,*P*,*P*-triphenylphosphinimidic chloride (PIN)

$(CH_3\text{-}CH_2)_2P(S)Cl$
diethylphosphinothioic chloride (PIN)

$C_6H_5\text{-}P(O)Cl_2$
phenylphosphonic dichloride (PIN)

$CH_3\text{-}CH_2\text{-}P(O)[N(CH_3)_2]Cl$
P-ethyl-*N*,*N*-dimethylphosphonamidic chloride (PIN)

$(CH_3)_2N\text{-}P(O)(NCO)Cl$
N,*N*-dimethylphosphoramidisocyanatidic chloride (PIN)

$HP(O)(NCO)_2$
phosphonic diisocyanate (PIN)

$P(=NH)(NCS)_3$
phosphorimidic triisothiocyanate (PIN)

$(CH_3)_2PN_3$
dimethylphosphinous azide (PIN)

$SO_2(NCO)_2$
sulfuryl diisocyanate (PIN)

$S(=N\text{-}CH_3)Cl_2$
N-methylsulfurimidous dichloride (PIN)

$F\text{-}SO_2\text{-}NCO$
sulfurisocyanatidic fluoride (PIN)

$F\text{-}S(=NH)(NCO)$
sulfurimidisocyanatidous fluoride (PIN)

$CH_3\text{-}NH\text{-}SO_2Cl$
N-methylsulfamoyl chloride (PIN)

P-67.1.2.5.2 Preferred IUPAC names of halides of the boron acids and silicic acid are substitutive names.

Examples:

$C_6H_5\text{-}B(Cl)(Br)$
bromo(chloro)(phenyl)borane (PIN)
phenylboronic bromide chloride
phenylboronobromidic chloride

$CH_3\text{-}SiCl_3$
trichloro(methyl)silane (PIN)

$SiCl_4$
tetrachlorosilane (preselected name)
silicon tetrachloride
(not silicic tetrachloride)

P-67.1.2.6 Amides and hydrazides

Amides and hydrazides are named by functional class nomenclature by replacing the term ‘acid’ in the name of the corresponding acid by ‘amide’ or ‘hydrazide’. Amides and hydrazides of nitric acid and nitrous acid are discussed in P-67.1.2.6.3. Preferred IUPAC names of amides and hydrazides of the boron acids and silicic acid are exceptions (see P-67.1.2.6.2) as are azorous acid, azinous acid and azonous acid which are names of polyazanes.

P-67.1.2.6.1 Preferred IUPAC names of amides and hydrazides are denoted by the class name ‘amide’ or ‘hydrazide’:

(a) when all –OH groups in the corresponding acid have been replaced by $–NH_2$ or $–NH\text{-}NH_2$ groups, and

(b) when the amide or hydrazide is the principal functional group in accordance with the following order of seniority:

Br, Cl, F, I, N_3, CN, NC, NCO, ONC, NH_2 (amide), $\overset{1}{N}H\overset{2}{N}H_2$ (hydrazide)

Note: This order is not quite the same as that used by CAS (where amide follows the halogens and precedes the pseudohalogens) but it is consistent with the order of compound classes in P-41.

Substituents on the nitrogen atoms are denoted by italic letter locants such as, *N* (primed and double primed as required), in addition to the italic letter locants ‘*P*’, ‘*As*’, and ‘*Sb*’.

Locants to denote hydrazides are 1 and 2, primed and double primed as required.

Examples:

$[(CH_3)_2N]_3PO$
hexamethylphosphoric triamide (PIN)
hexamethylphosphoramide
[not phosphoric tris(dimethylamide)]

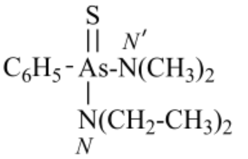
$(CH_3)_2P(O)[N(CH_3)_2]$
N,*N*,*P*,*P*-tetramethylphosphinic amide (PIN)
(not dimethylphosphinic dimethylamide)

$C_6H_5\text{-}P(O)(NHCH_3)_2$
N,*N′*-dimethyl-*P*-phenylphosphonic diamide (PIN)
[not phenylphosphonic bis(methylamide)]

$C_6H_5\text{-}P(S)[N(CH_3)_2]_2$
N,*N*,*N′*,*N′*-tetramethyl-*P*-phenylphosphonothioic diamide (PIN)

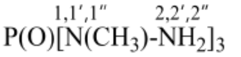
$C_6H_5\text{-}Sb(S)[N(CH_3)_2][N(CH_2\text{-}CH_3)_2]$
N,*N*-diethyl-*N′*,*N′*-dimethyl-*Sb*-phenylstibonothioic diamide (PIN)

$(CH_3)_2N\text{-}P(O)Cl_2$
N,*N*-dimethylphosphoramidic dichloride (PIN)



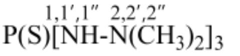
$$C_6H_5\text{-}\underset{\underset{\overset{N}{N}(CH_2\text{-}CH_3)_2}{|}}{\overset{\overset{S}{||}}{As}}\text{-}\overset{N'}{N}(CH_3)_2$$

N,*N*-diethyl-*N′*,*N′*-dimethyl-*As*-phenylarsonothioic diamide (PIN)



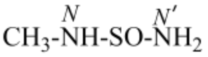
$$P(O)[\overset{1,1',1''}{N}(CH_3)\text{-}\overset{2,2',2''}{N}H_2]_3$$

1,1′,1″-trimethylphosphoric trihydrazide (PIN)



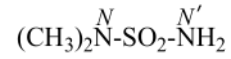
$$P(S)[\overset{1,1',1''}{N}H\text{-}\overset{2,2',2''}{N}(CH_3)_2]_3$$

2,2,2′,2′,2″,2″-hexamethylphosphorothioic trihydrazide (PIN)
[not phosphorothioic tris(2,2-dimethylhydrazide)]



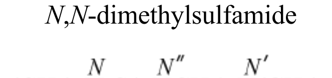
$$CH_3\text{-}\overset{N}{N}H\text{-}SO\text{-}\overset{N'}{N}H_2$$

N-methylsulfurous diamide (PIN)



$$(CH_3)_2\overset{N}{N}\text{-}SO_2\text{-}\overset{N'}{N}H_2$$

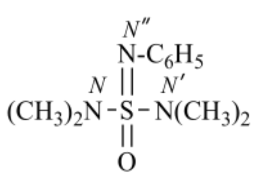
N,*N*-dimethylsulfuric diamide (PIN)
N,*N*-dimethylsulfamide



$$(CH_3)_2\overset{N}{N}\text{-}S(=\overset{N''}{N}CH_3)\text{-}\overset{N'}{N}(CH_3)_2$$

pentamethylsulfurimidous diamide (PIN)

$CH_3\text{-}NH\text{-}S(O)(=N\text{-}CH_3)\text{-}Br$
N,*N′*-dimethylsulfuramidimidic bromide (PIN)



$$(CH_3)_2\overset{N}{N}\text{-}\underset{\underset{O}{||}}{\overset{\overset{\overset{N''}{N}\text{-}C_6H_5}{||}}{S}}\text{-}\overset{N'}{N}(CH_3)_2$$

N,*N*,*N′*,*N′*-tetramethyl-*N″*-phenylsulfurimidic diamide (PIN)

P-67.1.2.6.2 Preselected names of amides and hydrazides of the boron acids and silicic acid are substitutive names based on the preselected parent hydride names borane and silane.

Examples:

$H_2B\text{-}NH_2$
boranamine

(name derived from the preselected name borane)
(not borinic amide)

$B(NH_2)_3$
boranetriamine
(name derived from the preselected name borane)
(not boric triamide)

$B(\overset{1,1',1''}{N}H-\overset{2,2',2''}{N}H_2)_3$
1,1′,1″-boranetriyltrihydrazine
(name derived from the preselected name borane)
(not boric trihydrazide)

$Si(NH_2)_4$
silanetetramine
(name derived from the preselected name silane)
(not silicic tetramide)

$Si(NH-NH_2)_4$
1,1′,1″,1‴-silanetetrayltetrahydrazine
(name derived from the preselected name silane)
(not silicic tetrahydrazide)

P-67.1.2.6.3 Amides and hydrazides of nitric and nitrous acids

Nitramines are amides of nitric acid (see ref. 23). The class is composed of ‘nitramide’ (a shortened form of nitric amide), NO_2-NH_2, and the names of its derivatives are formed by substitution. Nitrosamines are amides of nitrous acid, NO-NH_2 (see ref. 23); and the names of its derivatives are formed by substitution. Nitric acid and nitrous acid are preselected names, see P-12.

$O_2N\text{-}\overset{N}{N}H\text{-}\overset{N'}{N}H_2$
(I)

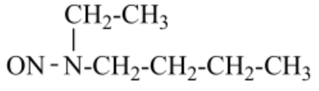
$ON\text{-}\overset{N}{N}H\text{-}\overset{N'}{N}H_2$
(II)

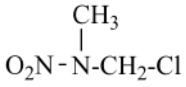
Similarly, nitric hydrazide (I) and nitrous hydrazide (II) are preselected names used as parent structures for generation of preferred IUPAC names.

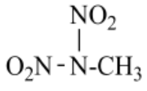
Preferred IUPAC names for amides and hydrazides of nitric and nitrous acids are now systematically based on nitric or nitrous amide and hydrazide, in accordance with the seniority order of classes rather than as nitro and nitroso amines; the latter names can be used in general nomenclature.

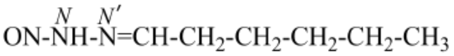
Examples:

$ON\text{-}N(CH_2\text{-}CH_2\text{-}CH_3)_2$
dipropylnitrous amide (PIN)
N-nitroso-*N*-propylpropan-1-amine


$ON\text{-}\overset{\overset{\displaystyle CH_2\text{-}CH_3}{|}}{N}\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}CH_3$
butyl(ethyl)nitrous amide (PIN)
N-ethyl-*N*-nitrosobutan-1-amine


$O_2N\text{-}\overset{\overset{\displaystyle CH_3}{|}}{N}\text{-}CH_2\text{-}Cl$
(chloromethyl)(methyl)nitramide (PIN)
1-chloro-*N*-methyl-*N*-nitromethanamine


$O_2N\text{-}\overset{\overset{\displaystyle NO_2}{|}}{N}\text{-}CH_3$
methyl(nitro)nitramide (PIN)
N,*N*-dinitromethanamine



$ON\text{-}\overset{N}{N}H\text{-}\overset{N'}{N}{=}CH\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}CH_3$

N′-hexylidenenitrous hydrazide (PIN)

P-67.1.3 Salts, esters, and anhydrides of mononuclear noncarbon oxoacids

The methodology discussed in this section is applicable to all mononuclear oxo acids whether or not they have retained names or names using infixes or prefixes.

P-67.1.3.1 Salts
P-67.1.3.2 Esters
P-67.1.3.3 Anhydrides

P-67.1.3.1 Salts of mononuclear noncarbon oxoacids

Neutral salts of mononuclear noncarbon oxoacids are named by citing the cation(s) followed by the name(s) of the anion(s) as a separate word. Names of anions are formed by changing the ‘ic acid’ ending to ‘ate’ and the ‘ous acid’ ending to ‘ite’. Different cations are cited in alphabetical order.

Examples:

$Na_2(CH_3\text{-}PO_2)$
disodium methylphosphonite (PIN)

$K[(CH_3)_2As(O)O]$
potassium dimethylarsinate (PIN)

Acid salts of polybasic mononuclear noncarbon oxoacids are named in the same way as neutral salts, the remaining acid hydrogen atom(s) being indicated by the word ‘hydrogen’ (or ‘dihydrogen’, etc., as appropriate) inserted between the name of the cation(s) and the name of the anion from which it is separated by spaces.

Note: In the nomenclature of inorganic chemistry (IR-8.4, ref. 12), the term ‘hydrogen’ is written directly in front of the name of the anion, without a space, to indicate that it is part of the anion.

Example:

$Na^+\ B(OH)(OCN)(O^-)$
sodium hydrogen borocyanatidate

P-67.1.3.2 Esters of mononuclear noncarbon oxoacids

Esters of mononuclear noncarbon acids are named in the same way as esters of organic acids (see P-65.6.3.2). Alkyl groups, aryl groups, etc. are cited as separate words, in alphanumerical order when more than one, and followed by the name of the appropriate anion. Partial acid esters of polybasic acids are named by citing alkyl groups, aryl groups, etc. as separate words, in alphanumeric order if more than one, followed by the word ‘hydrogen’ (with the appropriate multiplying prefix, as necessary) also cited as a separate word, and the name of the appropriate anion. Salts of partial acid esters are named by citing the name of the cation before the name of the organic group; remaining acids groups are denoted by the word ‘hydrogen’ as described above. Structural specificity for esters of chalcogen analogues of mononuclear noncarbon oxoacids is provided by the appropriate italic element symbols *O*, *S*, *Se*, and *Te*, prefixed to the name of the group, as needed.

Examples:

$CH_3\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}O\text{-}NO$
pentyl nitrite (PIN)

$CH_3\text{-}S\text{-}NO_2$
S-methyl thionitrate (PIN)

$(C_6H_5)_2P\text{-}O\text{-}CH_3$
methyl diphenylphosphinite (PIN)

$CH_3\text{-}P(Cl)(S\text{-}CH_2\text{-}CH_3)$
ethyl methylphosphonochloridothioite (PIN)

$CH_3\text{-}P(NH\text{-}CH_3)(OCH_3)$
methyl *N*,*P*-dimethylphosphonamidite (PIN)

$P(O\text{-}CH_3)_3$
trimethyl phosphite (PIN)

$P(Cl)[N(CH_3)_2](O\text{-}CH_3)$
methyl *N*,*N*-dimethylphosphoramidochloridite (PIN)

$P(O)(O\text{-}CH_3)_3$
trimethyl phosphate (PIN)

$P(O)(O\text{-}C_2H_5)(O\text{-}CH_3)(O\text{-}C_6H_5)$
ethyl methyl phenyl phosphate (PIN)

$P(O)(O\text{-}CH_3)(OH)_2$
methyl dihydrogen phosphate (PIN)

$C_6H_5\text{-}HAs(S)(O\text{-}CH_3)$
O-methyl phenylarsinothioate (PIN)

$CH_3\text{-}O\text{-}P(O)(OH)\text{-}O^- \ Na^+$
sodium methyl hydrogen phosphate (PIN)

$HP(O)(O\text{-}CH_3)_2$
dimethyl phosphonate (PIN)

$(CH_3\text{-}CH_2)_2P(S)(S\text{-}CH_2\text{-}CH_3)$
ethyl diethylphosphinodithioate (PIN)

$(CH_3)_2As(O)(S\text{-}CH_3)$
S-methyl dimethylarsinothioate (PIN)

$CH_3\text{-}P(O)(O\text{-}CH_2\text{-}CH_3)_2$
diethyl methylphosphonate (PIN)

$C_6H_5\text{-}P(O)(O\text{-}CH_3)(S\text{-}CH_2\text{-}CH_3)$
S-ethyl *O*-methyl phenylphosphonothioate (PIN)

$C_6H_5\text{-}P(O)(Cl)(O\text{-}CH_3)$
methyl phenylphosphonochloridate (PIN)

$(CH_3)_2N\text{-}P(O)(O\text{-}CH_3)_2$
dimethyl *N*,*N*-dimethylphosphoramidate (PIN)

$(CH_3\text{-}CH_2)_2N\text{-}P(O)(NCS)(O\text{-}CH_2\text{-}CH_3)$
ethyl *N*,*N*-diethylphosphoramid(isothiocyanatidate) (PIN)

$As(O)(F)(O\text{-}CH_3)_2$
dimethyl arsorofluoridate (PIN)

$Sb(O)(F)_2(S\text{-}CH_3)$
S-methyl stiborodifluoridothioate (PIN)

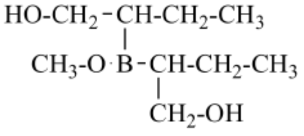
$(CH_3)_2B\text{-}O\text{-}C_6H_5$
phenyl dimethylborinate (PIN)

$CH_3\text{-}O\text{-}SO_2\text{-}OH$
methyl hydrogen sulfate (PIN)

$C_6H_5\text{-}O\text{-}F$
phenyl hypofluorite (PIN)

$CH_3\text{-}S\text{-}Cl$
methyl thiohypochlorite (PIN)

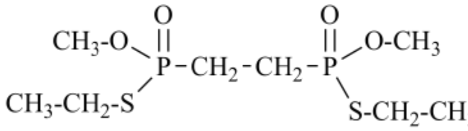
$CH_3\text{-}CO\text{-}CH_2\text{-}CH_2\text{-}O\text{-}BrO_2$
3-oxobutyl bromate (PIN)



$$\begin{array}{lllll} HO\text{-}CH_2\text{-} & CH\text{-}CH_2\text{-}CH_3 & & \\ & | & & \\ CH_3\text{-}O\text{-} & B & \text{-}CH\text{-}CH_2\text{-}CH_3 \\ & & \ \ | & \\ & & CH_2\text{-}OH & \end{array}$$

methyl bis(1-hydroxybutan-2-yl)borinate (PIN)

$Si(S\text{-}CH_3)_3(O\text{-}CH_2\text{-}CH_3)$
O-ethyl *S*,*S*,*S*-trimethyl trithiosilicate (PIN)



S,*S*′-diethyl *O*,*O*′-dimethyl *P*,*P*′-(ethane-1,2-diyl)bis(phosphonothioate)(PIN)

P-67.1.3.3 Anhydrides of mononuclear noncarbon oxoacids

Neutral anhydrides formed between acids named by suffixes and mononuclear noncarbon oxoacids described in P-67.1.1 are named in the same way as described for anhydrides derived from carboxylic and the sulfur acids named by suffixes (see P-65.7). The names of the acids are cited in alphabetical order followed by the class name 'anhydride' prefixed by a numerical term indicating the number of anhydride linkages (the numerical prefix mono is not used); such names lead to preferred IUPAC names. Names formed by acyl groups substituting the phosphorus, arsenic or antimony mononuclear oxoacid modified by the ending 'ate' can be used in general nomenclature. Halogen oxoacids form anhydrides with carboxylic and the sulfur acids expressed by suffixes.

Acidic anhydrides are named as described in P-67.3.1 using the senior acid as parent, or by using systematic substitutive nomenclature.

Examples:

$(CH_3)_2B\text{-}O\text{-}CO\text{-}CH_3$
acetic dimethylborinic anhydride (PIN)

$CH_3\text{-}CO\text{-}O\text{-}As(O)(CH_3)_2$
acetic dimethylarsinic anhydride (PIN)
acetyl dimethylarsinate

$B(O\text{-}CO\text{-}CH_3)_3$
acetic boric trianhydride (PIN)

$[(CH_3)_2CH]_2Sb\text{-}S\text{-}C(S)\text{-}N(CH_2\text{-}CH_3)_2$
diethylcarbamothioic di(propan-2-yl)stibinous thioanhydride (PIN)

$C_6H_5\text{-}CO\text{-}O\text{-}I$
benzoic hypoiodous anhydride (PIN)

$(CH_3)_2B\text{-}O\text{-}O\text{-}B(CH_3)_2$
dimethylborinic peroxyanhydride (PIN)

$B(OCN)_3$
boric cyanic trianhydride (PIN)

$CH_3\text{-}HP(O)(OCN)$
cyanic methylphosphinic anhydride (PIN)

P-67.1.4 Substituent prefix groups derived from mononuclear noncarbon oxoacids

P-67.1.4.1 Substituent groups derived from the mononuclear nitrogen, phosphorus, arsenic, and antimony acids
P-67.1.4.2 Substituent groups derived from boron acid and silicic acid
P-67-1.4.3 Substituent groups derived from nitric and nitrous acids
P-67.1.4.4 Substituent groups derived from chalcogen acids
P-67.1.4.5 Substituent groups derived from halogen acids

P-67.1.4.1 Substituent groups derived from the mononuclear nitrogen, phosphorus, arsenic, and antimony acids

P-67.1.4.1.1 Preselected prefixes
P-67.1.4.1.2 Substituent groups for general nomenclature
P-67.1.4.1.3 Compound and complex substituent groups

P-67.1.4.1.1 Preselected prefixes.

Substituent prefix groups derived from mononuclear noncarbon oxoacids have retained names and systematic names corresponding to simple or compound acyl groups. The preselected prefixes are formed by applying the following seniority order, in the order given, until a decision is reached:

P-67.1.4.1.1.1 Retained names for substituent groups derived from mononuclear noncarbon oxoacids;
A few names denoting monovalent acidic groups are retained. These names are preselected names when unsubstituted or for chalcogen analogues when the position of chalcogen atoms introduced by functional replacement is not known or it is not necessary to specify their position(s): the chalcogen atoms are expressed by prefixes.

Acid	Derived preselected prefix
$-N(O)(OH)_2$	azono (preselected prefix)
$-P(O)(OH)_2$	phosphono (preselected prefix)
$-As(O)(OH)_2$	arsono (preselected prefix)
$-Sb(O)(OH)_2$	stibono (preselected prefix)
$-P(O)(OH)(SH)$ or $-P(S)(OH)_2$	thiophosphono (preselected prefix)
$-P(S)(SH)_2$	trithiophosphono (preselected prefix)

P-67.1.4.1.1.2 Fundamental acyl groups for substituents derived from mononuclear noncarbon oxoacids;

Acyl prefix groups are formed by removing all –OH groups from a mononuclear noncarbon oxoacid having the general structures $E(=O)(OH)_3$, $R-E(=O)(OH)_2$ or $R,R'E(=O)OH$, where R and R′ = H or an organyl group. Names of acyl groups derived from the names of acids, modified or not by functional replacement, by elimination of all hydroxy groups or their chalcogen analogues, are formed by changing the ‘ic acid’ ending in the name of the acid to ‘oyl’, with the exception of ‘nitroryl’ $-N(O)<$; ‘phosphoryl’, $-P(O)<$; ‘arsoryl’, $-As(O)<$; and ‘stiboryl’, $-Sb(O)<$. Prefixes formed in this manner are preselected prefixes. For example, the group ‘phosphoryl’ $-P(O)<$, is derived from phosphoric acid, $P(O)(OH)_3$ or phosphorothioic *S*-acid, $P(O)(OH)_2(SH)$, or phosphorodithioic *S*,*S*-acid, $P(O)(SH)_2(OH)$ or phosphorotrithioic *S*,*S*,*S*-acid, $P(O)(SH)_3$.

The prefix ‘nitroryl’ (not azoryl), for the acyl group $-N(O)<$, derived from the hypothetical nitroric acid, $N(O)(OH)_3$, has been recommended since 1993 (see R-3.3, ref. 2).

Examples:

Acid		Derived preselected prefix	
$N(O)(OH)_3$	nitroric acid (hypothetical; preselected name)	$-N(O)<$	nitroryl (preselected prefix)
$P(O)(OH)_3$	phosphoric acid (preselected name)	$-P(O)<$	phosphoryl (preselected prefix)
$As(O)(OH)_3$	arsoric acid (preselected name) (not arsenic acid)	$-As(O)<$	arsoryl (preselected prefix) (not arsenyl)
$Sb(O)(OH)_3$	stiboric acid (preselected name) (not antimonic acid)	$-Sb(O)<$	stiboryl (preselected prefix) (not antimonyl)
$NH(O)(OH)_2$	azonic acid (preselected name)	$NH(O)<$	azonoyl (preselected prefix)
$NH_2(O)(OH)$	azinic acid (preselected name)	$NH_2(O)-$	azinoyl (preselected prefix)
$PH(O)(OH)_2$	phosphonic acid (preselected name)	$PH(O)<$	phosphonoyl (preselected prefix)
$PH_2(O)(OH)$	phosphinic acid (preselected name)	$PH_2(O)-$	phosphinoyl (preselected prefix) (not phosphinyl)
$AsH(O)(OH)_2$	arsonic acid (preselected name)	$AsH(O)<$	arsonoyl (preselected prefix)
$AsH_2(O)OH$	arsinic acid (preselected name)	$AsH_2(O)-$	arsinoyl (preselected prefix (not arsinyl)
$SbH(O)(OH)_2$	stibonic acid (preselected name)	$SbH(O)<$	stibonoyl (preselected prefix)
$SbH_2(O)OH$	stibinic acid (preselected name)	$SbH_2(O)-$	stibinoyl (preselected prefix)

P-67.1.4.1.1.3 Names of substituted fundamental acyl groups derived from mononuclear noncarbon oxoacids

Names of substituted fundamental acyl groups are formed directly from those of the acids generated by the method described in P-67.1.4.1.1.2. Preferred prefix names of acyl groups are those derived from the preferred IUPAC names of acids. The addition of hydrogen atoms to acyl groups by the method of concatenation, described in P-67.1.4.1.2, is not allowed.

Examples:

Acid	Derived preferred prefix
$CH_3-P(O)(OH)_2$ methylphosphonic acid (PIN)	$CH_3-P(O)<$ methylphosphonoyl (preferred prefix)
$CH_3-CH_2-SbH(O)OH$ ethylstibinic acid (PIN)	$CH_3-CH_2-SbH(O)-$ ethylstibinoyl (preferred prefix)
$C_6H_5-As(CH_3)(O)OH$ methyl(phenyl)arsinic acid (PIN)	$C_6H_5-As(CH_3)(O)-$ methyl(phenyl)arsinoyl (preferred prefix)

P-67.1.4.1.1.4 Names of acyl groups derived from mononuclear noncarbon oxoacids modified by functional replacement nomenclature

Preferred IUPAC prefixes are formed by the methodology indicated in P-65.2.1.5 for acyl groups derived from carbonic acids modified by the infixes and prefixes in functional replacement nomenclature. All infixes and prefixes listed in Table 1.6 and cited in P-65.1.2.3 are allowed. Applied to the B, N, P, As and Sb mononuclear noncarbon oxoacids, the method consists of first achieving functional replacement in acids, then removing all remaining –OH groups. Preselected names use infixes to denote functional replacement. Names using prefixes to effect functional replacement may be used in general nomenclature.

Examples:

Acid	**Derived preselected or preferred prefix**
$P(S)(OH)_3$ phosphorothioic *O*,*O*,*O*-acid (preselected name) thiophosphoric *O*,*O*,*O*-acid	$>P(S)–$ phosphorothioyl (preselected prefix) thiophosphoryl
$As(=NH)(OH)_3$ arsorimidic acid (preselected name) imidoarsoric acid	$>As(=NH)–$ arsorimidoyl (preselected prefix) imidoarsoryl
$Sb(=NNH_2)(OH)_3$ stiborohydrazonic acid (preselected name) hydrazonostiboric acid	$>Sb(=NNH_2)–$ stiborohydrazonoyl (preselected prefix) hydrazonostiboryl
$NH(S)(OH)_2$ azonothioic acid (preselected name) thioazonic acid	$>NH(S)$ azonothioyl (preselected prefix) thioazonoyl
$PH_2(=NH)(OH)$ phosphinimidic acid (preselected name) imidophosphinic acid	$–PH_2(=NH)$ phosphinimidoyl (preselected prefix) imidophosphinoyl
$(CH_3)_2P(Se)(OH)$ dimethylphosphinoselenoic acid (PIN) dimethyl(selenophosphinic acid)	$(CH_3)_2P(Se)–$ dimethylphosphinoselenoyl (preferred prefix) dimethyl(selenophosphinoyl)
$C_6H_5\text{-}P(O)Cl(OH)$ phenylphosphonochloridic acid (PIN) phenyl(chlorophosphonic acid)	$C_6H_5\text{-}P(O)(Cl)–$ phenylphosphonochloridoyl (preferred prefix) phenyl(chlorophosphonoyl)
$P(\equiv N)(OH)_2$ phosphoronitridic acid (preselected name) nitridophosphoric acid	$>P(\equiv N)$ phosphoronitridoyl (preselected prefix) nitridophosphoryl
$P(=NH)(NHNH_2)(OH)_2$ phosphorohydrazidimidic acid (preselected name) hydrazidimidophosphoric acid	$>P(=NH)(NHNH_2)$ phosphorohydrazidimidoyl (preselected prefix) hydrazidimidophosphoryl
$P(O)Cl_2(OH)$ phosphorodichloridic acid (preselected name) dichlorophosphoric acid	$P(O)(Cl)_2–$ phosphorodichloridoyl (preselected prefix) dichlorophosphoryl
$(CH_3)_2N\text{-}P(O)(OH)_2$ *N*,*N*-dimethylphosphoramidic acid (PIN) (dimethylamido)phosphoric acid	$(CH_3)_2N\text{-}P(O)<$ *N*,*N*-dimethylphosphoramidoyl (preferred prefix) (dimethylamido)phosphoryl
$P(O)(OH)_2(OOH)$ phosphoroperoxoic acid (preselected prefix) peroxyphosphoric acid	$>P(O)(OOH)$ phosphoroperoxoyl (preselected prefix) (hydroperoxy)phosphoryl peroxyphosphoryl
$P(O)(OH)_2(OSH)$ or $P(O)(OH)_2(SOH)$ phosphoro(thioperoxoic) acid (preselected name) (thioperoxy)phosphoric acid	$>P(O)(OSH)$ or $>P(O)(SOH)$ phosphoro(thioperoxoyl) (preselected prefix) (thiohydroperoxy)phosphoryl

P-67.1.4.1.1.5 Names for preferred or preselected prefixes of acyl groups substituted by hydroxy groups or their chalcogen and peroxy analogues.

Concatenation is the recommended method to reintroduce groups and their chalcogen analogues in substituent groups or groups that are not treated as infixes in functional replacement nomenclature, such as '–OR', '–SR', etc. It is important to respect the concatenation procedure that is an additive operation using acyl groups only. The following acyl groups are allowed: basic acyl groups described in P-67.1.4.1.1.2 above, substituted basic acyl groups described in P-67.1.4.1.1.3 above, and acyl groups modified by functional replacement described in P-67.1.4.1.1.4 above. Substitution of hydrogen atoms attached to the central atom (substitutable hydrogen) in the basic acyl groups described in P-67.1.4.1.1.2 above is not allowed to generate preferred IUPAC names.

This method is not recommended to generate any of the prefixes in P-67.1.4.1.1.1 above.

Examples:

$-NH(O)(OH)$
hydroxyazonoyl (preselected prefix)

$-P(Se)(OCH_3)_2$
dimethoxyphosphoroselenoyl (preferred prefix)
dimethoxy(selenophosphoryl)

$-P(O)(OH)(SH)$
hydroxy(sulfanyl)phosphoryl (preselected prefix)

$-P(O)(SH)_2$
bis(sulfanyl)phosphoryl (preselected prefix)

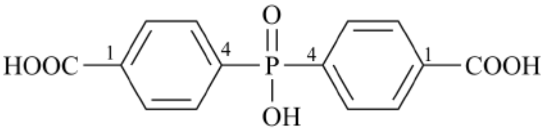
$-PH(O)(SeH)$
selanylphosphonoyl (preselected prefix)

$-PH(S)(SH)$
sulfanylphosphonothioyl (preselected prefix)
sulfanyl(thiophosphonoyl)

$>P(O)(OSH)$
(sulfanyloxy)phosphoryl (preselected prefix)
(*SO*-thiohydroperoxy)phosphoryl

$>P(S)(SOH)$
(hydroxysulfanyl)phosphorothioyl (preselected prefix)
(*OS*-thiohydroperoxy)phosphorothioyl

$CH_3-P(O)(OH)-$
hydroxy(methylphosphonoyl) (preferred prefix)



4,4′-(hydroxyphosphoryl)dibenzoic acid (PIN)

P-67.1.4.1.1.6 Substitutive names for groups derived from mononuclear noncarbon oxoacids

Substitutive nomenclature based on parent hydrides BH_3, PH_3, AsH_3, SbH_3, PH_5, AsH_5, SbH_5 is used to generate names of substituent groups for which acyl group names cannot be generated by the methods in P-67.1.4.1.1.1 through P-67.1.4.1.1.5 and the corresponding As and Sb acids. It is also used to indicate a different type of free valencies, for example an ‘ylidene’ type instead of the ‘diyl’ observed in a substituent group derived from the acid in criteria (b) and (d).

Examples:

$-P(OH)_2$
dihydroxyphosphanyl (preselected prefix)

$-AsH(OH)$
hydroxyarsanyl (preselected prefix)

$-AsHCl$
chloroarsanyl (preselected prefix)

$-P(NH_2)_2$
diaminophosphanyl (preselected prefix)

$>Sb(OH)$
hydroxystibanediyl (preselected prefix)

$=P(OH)$
hydroxyphosphanylidene (preselected prefix)

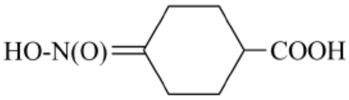
$=B(O-CH_3)$
methoxyboranylidene (preferred prefix)

$-P(O-CH_3)_2$
dimethoxyphosphanyl (preferred prefix)

=P(O)(OH)
hydroxy(oxo)-λ^5-phosphanylidene (preselected prefix)

=As(O)(OCH$_3$)
methoxy(oxo)-λ^5-arsanylidene (preferred prefix)

=N(O)OH
hydroxy(oxo)-λ^5-azanylidene (preselected prefix)
aci-nitro
(see P-67.1.6)



4-[hydroxy(oxo)-λ^5-azanylidene]cyclohexane-1-carboxylic acid (PIN)
4-*aci*-nitrocyclohexane-1-carboxylic acid
(see *aci*-nitro compounds, P-67.1.6)

–P=O
oxophosphanyl (preselected prefix)

–P(O)$_2$
dioxo-λ^5-phosphanyl (preselected prefix)

–Sb=O
oxostibanyl (preselected prefix)

P-67.1.4.1.2 Substituent groups for general nomenclature

The prefix ‘hydro’ may be added by concatenation only for use in general nomenclature.

Examples:

>PH(O)
hydrophosphoryl
phosphonoyl (preselected prefix)

>PH(S)
hydro(thiophosphoryl)
phosphonothioyl (preselected prefix)

P-67.1.4.1.3 Compound and complex substituent groups

If a B, N, P, As, or Sb containing group is attached by an oxygen or other chalcogen atom or a nitrogen atom to a compound that also contains another substituent having priority over the B, N, P, As, or Sb containing group for citation as principal group, then the B, N, P, As, or Sb containing group is named by a compound or complex prefix built from prefixes described above and arranged in the order in which the components occur in the compound.

Examples:

(HO)$_2$P(O)-O-CH$_2$-COOH
(phosphonooxy)acetic acid (PIN)

(CH$_3$O)$_2$P(O)-S-CH$_2$-CH$_2$-COOH
3-[(dimethoxyphosphoryl)sulfanyl]propanoic acid (PIN)

(HO)(HS)P(S)-NH-CH$_2$-CH$_2$-COOH
3-{[hydroxy(sulfanyl)phosphorothioyl]amino}propanoic acid (PIN)

P-67.1.4.2 Substituent groups derived from the boron acids and silicic acid

Substituent groups derived from boron and silicon mononuclear acids and their analogues are formed by substituting the parent hydride names ‘borane’ and ‘silane’. The name borono, for –B(OH)$_2$, is retained and is the preselected name.

The name boryl has been used for the substituent group H$_2$B–, now named boranyl as the preselected name, and consequently is not to be used for the prefix group derived from boric acid by removal of all three –OH groups.

Examples:

–B(OH)$_2$
borono (preselected prefix)

$–BH_2$
boranyl (preselected prefix)
(not boryl)

$>BH$
boranediyl (preselected prefix)
(not boronoyl)

$–B<$
boranetriyl (preselected prefix)
(not boryl)

$=BH$
boranylidene (preselected prefix)
(not boronoyl)

$≡B$
boranylidyne (preselected prefix)
(not boryl)

$–B(NH_2)_2$
diaminoboranyl (preselected prefix)
(not borodiamidoyl)

$–BH(O\text{-}CH_3)$
methoxyboranyl (preferred prefix)
(not hydromethoxyboryl)

$–Si(OH)_3$
trihydroxysilyl (preselected prefix)

$–SiCl_2(NH_2)$
aminodichlorosilyl (preselected prefix)

$–Si(O\text{-}CH_3)_3$
trimethoxysilyl (preferred prefix)

$–Si(OH)_2(SH)$
dihydroxy(sulfanyl)silyl (preselected prefix)

P-67.1.4.3 Substituent groups derived from nitric acid and nitrous acid

The acyl groups ‘nitro’ for $–NO_2$ and ‘nitroso’ for –NO when attached to the following elements C, P, As, Sb, Bi, Si, Ge, Sn, Pb, B, Al, Ga, In, and Tl were discussed in P-61.5. In this section, the rules for naming substituent groups related to esters, amides and hydrazides of nitric acid and nitrous acid are discussed.

P-67.1.4.3.1 Substituent groups derived from esters of nitric acid and nitrous acid

Nitrates and nitrites as esters of nitric acid and nitrous acid are discussed in P-67.1.3.2. Substituent groups derived from these compounds are named by concatenation by adding the acyl groups ‘nitro’ for $–NO_2$ and ‘nitroso’ for –NO to the prefix ‘oxy’ or by substituting these acyl groups into substituent groups such as ‘sulfanyl’ , ‘selanyl’, or ‘tellanyl’.

Examples:

$–O\text{-}NO_2$
nitrooxy (preselected prefix)

$–S\text{-}NO_2$
nitrosulfanyl (preselected prefix)

–O-NO
nitrosooxy (preselected prefix

–Se-NO
nitrososelanyl (preselected prefix)

P-67.1.4.3.2 Substituent groups derived from amides of nitric acid and nitrous acid

The amide of nitric acid, $O_2N\text{-}NH_2$, is named ‘nitramide’ and the substituent group derived from this amide by the loss of one hydrogen atom is called ‘nitramido’ by applying the general rule for naming amides (see P-66.1.1.4.3); that is, changing the final letter ‘e’ of the amide name to ‘o’. Other derivatives and those derived from nitrous amide, $ON–NH_2$, are formed by substituting the acyl groups ‘nitro’ and ‘nitroso’ into the appropriate substituent groups ‘amino’, ‘imino’, and ‘azanetriyl’. It must be noted that the location of the groups –NO and $-NO_2$ to another nitrogen atom does not constitute lengthening of a chain.

Examples:

–NH-NO
nitrosoamino (preselected prefix)

$>N\text{-}NO_2$
nitroazanediyl (preselected prefix)

$=N\text{-}NO_2$
nitroimino (preselected prefix)

$-NH\text{-}NO_2$
nitramido (preselected prefix)

–N=S
sulfanylideneamino (preselected prefix)
thioxoamino
thionitroso

$-O_2S\text{-}N{=}S$
(sulfanylideneamino)sulfonyl (preselected prefix)
(thioxoimino)sulfonyl
(thionitroso)sulfonyl

P-67.1.4.3.3 Substituent groups derived from the hydrazides of nitric acid and nitrous acid

Substituent groups derived from nitric hydrazide, $O_2N\text{-}NH\text{-}NH_2$, and nitrous hydrazide, $ON\text{-}NH\text{-}NH_2$, are named by substituting the acyl groups ‘nitro’ or ‘nitroso’ into the appropriate substituent group ‘hydrazin-1-yl’, ‘hydrazin-1-ylidene’, etc.

Examples:

$O_2N\text{-}\overset{2}{N}H\text{-}\overset{1}{N}H\text{–}$
2-nitrohydrazin-1-yl (preselected prefix)

$ON\text{-}\overset{2}{N}H\text{-}\overset{1}{N}{=}$
nitrosohydrazinylidene (preselected prefix)

$H_2\overset{2}{N}\text{-}\overset{1}{N}(NO_2)\text{–}$
1-nitrohydrazin-1-yl (preselected prefix)

P-67.1.4.4 Substituent groups derived from chalcogen acids

P-67.1.4.4.1 Acyl groups

There are two methods to generate names of acyl groups derived from the chalcogen acids for use as substituent groups.

(1) The methodology described in P-65.3.2.3, i.e., infixes denoting functional replacement by -S-, -Se-, -Te-, =NH, and $=NNH_2$, and concatenation for other atoms or groups.

(2) The general method described in P-65.2.1.5 for deriving acyl groups from derivatives of carbonic acid, and applied in P-67.1.4.1.1.4 for acyl groups derived from phosphoric, phosphonic and phosphinic acids and their arsenic and antimony congeners is applied to sulfuric acid and its functional replacement analogues.

Method (1) produces preselected prefixes.

Examples:

$-SO_2-$
sulfonyl (preselected prefix)
sulfuryl

–S(O)(S)–
sulfonothioyl (preselected prefix)
sulfurothioyl

$–S(S)_2–$
sulfonodithioyl (preselected prefix)
sulfurodithioyl

$–S(O)(=NH)–$
sulfonimidoyl (preselected prefix)
sulfurimidoyl

$–S(=NH)_2–$
sulfonodiimidoyl (preselected prefix)
sulfurodiimidoyl

$–S(O)(=NNH_2)–$
sulfonohydrazonoyl (preselected prefix)
sulfurohydrazonoyl

$–S(=NNH_2)_2–$
sulfonodihydrazonoyl (preselected prefix)
sulfurodihydrazonoyl

$–SO_2\text{-}Cl$
chlorosulfonyl (preselected prefix)
sulfurochloridoyl

$–SO_2\text{-}CN$
cyanosulfonyl (preferred prefix)
sulfurocyanidoyl

$–SO_2\text{-}NCS$
isothiocyanatosulfonyl (preferred prefix)
sulfur(isothiocyanatidoyl)

$–S(O)(S)\text{-}NCS$
isothiocyanatosulfonothioyl (preferred prefix)
sulfur(isothiocyanatido)thioyl

$–SO_2\text{-}O\text{-}CH_3$
methoxysulfonyl (preferred prefix)
methoxysulfuryl

$–S(=O)\text{-}Cl$
chlorosulfinyl (preselected prefix)

Method (2) cannot be applied to sulfurous acid, selenic acid and selenous acid, and telluric acid and tellurous acid, because ambiguous names may result.

P-67.1.4.4.2 If a sulfur-containing group is attached by oxygen (chalcogen) or nitrogen to a compound that contains also another substituent having priority over the sulfur- containing group for citation as principal group, then the sulfur-containing group is named by an appropriate prefix formed by concatenation or substitution (see P-35.4) as described in P-65.3.2.3 and P-67.1.4.4.1.

Examples:

$HO\text{-}SO_2\text{-}O\text{-}\overset{3}{C}H_2\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}OOH$
3-(sulfooxy)propanoic acid (PIN)

$CH_3\text{-}O\text{-}SO\text{-}O\text{-}\overset{3}{C}H_2\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}OOH$
3-[(methoxysulfinyl)oxy]propanoic acid (PIN)

$Cl\text{-}SO_2\text{-}O\text{-}\overset{3}{C}H_2\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}OOH$
3-[(chlorosulfonyl)oxy]propanoic acid (PIN)
3-(sulfurochloridoyloxy)propanoic acid

$H_2N\text{-}SO_2\text{-}O\text{-}\overset{3}{C}H_2\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}OOH$
3-(sulfamoyloxy)propanoic acid (PIN)
3-(sulfuramidoyloxy)propanoic acid
[not 3-(sulfonamidoyloxy)propanoic acid;
the name sulfonamidic acid is not an approved name]

$$H_2N\text{-}SO\text{-}O\text{-}\overset{3}{C}H_2\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}OOH$$

3-[(aminosulfinyl)oxy]propanoic acid (PIN)
[not 3-(sulfinamidoyloxy)propanoic acid;
the name sulfinamidic acid is not an approved name]

$$CH_3\text{-}O\text{-}SO_2\text{-}NH\text{-}\overset{3}{C}H_2\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}OOH$$

3-[(methoxysulfonyl)amino]propanoic acid (PIN)

P-67.1.4.5 Substituent groups derived from halogen acids

Names of prefixes derived from halogen acids and their chalcogen analogues are used as compulsory prefixes in substitutive nomenclature. They are listed in Table 5.1 and discussed in P-61.3.2.3.

Examples:

$OCl–$
chlorosyl (preselected prefix)

$SCl–$
thiochlorosyl (preselected prefix)

$O_2Cl–$
chloryl (preselected prefix)

$O_3Cl–$
perchloryl (preselected prefix)

The corresponding Br , F and I groups are named in a similar manner.

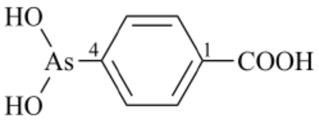
Example:

$C_6H_5\text{-}BrO$
bromosylbenzene (PIN)

P-67.1.5 Seniority order among noncarbon oxoacids and derivatives

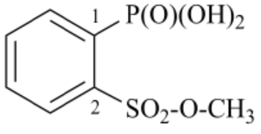
P-67.1.5.1 When a characteristic group having priority to be cited as principal group is present (see seniority order of classes, P-41, and of acids, P-42), prefixes having retained names or names systematically formed (see P-67.1.4.1) are used to denote inorganic acids.

Examples:



4-(dihydroxyarsanyl)benzoic acid (PIN)
[$–COOH$ is senior to $–As(OH)_2$]

$(HO)_2P(O)\text{-}CH_2\text{-}COOH$
phosphonoacetic acid (PIN)



[2-(methoxysulfonyl)phenyl]phosphonic acid (PIN)
(an acid is senior to an ester)

$$(HO)_2As(O)\text{-}\overset{4}{C}H_2\text{-}\overset{3}{C}H_2\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}H_2\text{-}P(O)(OH)_2$$

(4-arsonobutyl)phosphonic acid (PIN)
(a phosphorus acid is senior to an arsenic acid)

$C_6H_5\text{-}SO_2\text{-}N{=}P(NH\text{-}C_6H_5)_3$
N-(trianilino-λ^5-phosphanylidene)benzenesulfonamide (PIN)
N-(trianilinophosphoranylidene)benzenesulfonamide
[not *N*,*N*′,*N*″-triphenyl-*N*‴-benzenesulfonylphosphorimidic triamide;
nor *N*‴-benzenesulfonylphosphorimidic tris(phenylamide)]

P-67.1.5.2 When derivatives of mononuclear acids are named by functional class nomenclature, the seniority order is established in accordance with the greater number of atoms linked to the central atom and appearing as early as possible in the list: O, OO, S, Se, Te for the acids, then F, Cl, Br, I, then the pseudohaliodes in the order N_3, CN, NC, NCO, NCS, NCSe, NCTe, then amides and hydrazides.

Examples:

$Br_2P(O)-CH_2-CH_2-P(O)Cl_2$
(2-phosphorodibromidoylethyl)phosphonic dichloride (PIN)
(Cl is senior to Br in the seniority order of classes)

$Br_2P(O)-CH_2-CH_2-P(S)Cl_2$
(2-phosphorodichloridothioylethyl)phosphonic dibromide (PIN)
(phosphonic dibromide is preferred to phosphonothioic dichloride;
O > S is considered before Cl > Br)

$Cl_2P(O)-O-CH_2-CH_2-O-P(O)Cl(NH_2)$
2-(phosphoramidochloridoyloxy)ethyl phosphorodichloridate (PIN)
(phosphorodichloridic acid preferred to phosphoramidochloridic acid)

P-67.1.6 *aci*-Nitro compounds

aci-Nitro compounds deserve a special mention. They are tautomers of nitro compounds having the general structure $R=N(O)OH$ or $R_2N(O)OH$ and are named as derivatives of azinic acid, $H_2N(O)OH$.

Example:

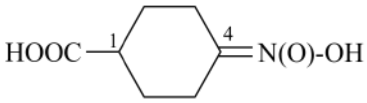
$CH_2=N(O)-OH$
methylideneazinic acid (PIN)
aci-nitromethane

When needed, the $R_2N(O)–$ group is designated by a prefix derived from 'azinoyl', that is preferred to 'nitroryl' (see P-67.1.4.1.1.2). The group $=N(O)OH$ is named 'hydroxy(oxo)-λ^5-azanylidene'.

The name 'hydroxy(oxo)-λ^5-azanylidene' is a change from the 1993 (ref. 2) recommended name 'hydroxynitroryl', that is not acceptable in the context of these recommendations where two free valencies must be expressed by the correct 'ylidene' or 'diyl' type.

Examples:

$(CH_3)_2N(O)-CH_2-CN$
cyano-*N*,*N*-dimethylmethanamine *N*-oxide (PIN; see P-62.5)
(dimethylazinoyl)acetonitrile
[not (dimethylnitroryl)acetonitrile]



4-[hydroxy(oxo)-λ^5-azanylidene]cyclohexane-1-carboxylic acid (PIN)
4-*aci*-nitrocyclohexane-1-carboxylic acid

P-67.2 DI- AND POLYNUCLEAR NONCARBON OXOACIDS

Like mononuclear acids, polynuclear acids have retained names that are used as preselected names. Substitutive or additive names are not recommended. Retained names are used as parents and are modifiable by functional replacement in the same manner that mononuclear acids are, except that only prefixes are used for the functional replacement operation.

Di- and polynuclear noncarbon oxoacids, whose central atoms are B, P, As, Sb, S, Se, are described here. They are divided into three types. Di- and trinuclear acids are exemplified for each central atom. In some cases higher polynuclear acids are known. Their names are formed by using the appropriate multiplying prefixes to indicate the number of central atoms. Di- and polynuclear noncarbon oxoacids are discussed in Sections P-67.2 and P-67.3.

Insofar as their structures are known and conform to those of the phosphorus acids, arsenic and antimony acids are named in the same way as those of phosphorus, with 'ars' and 'stib', respectively, in place of 'phosph'. Similarly, tellurium acids are named in the same way as those of selenium, by changing 'selen' to 'tellur' in the names of acids.

P-67.2.1 Preselected names
P-67.2.2 Functional replacement derivatives of di- and polynuclear noncarbon oxoacids
P-67.2.3 Acid halides and pseudohalides of di- and polynuclear noncarbon oxoacids
P-67.2.4 Amides and hydrazides of di- and polynuclear noncarbon oxoacids

P-67.2.5 Esters and anhydrides of di- and polynuclear noncarbon oxoacids
P-67.2.6 Substituent groups derived from polyacids

P-67.2.1 Preselected names

The following traditional names are retained as preselected names (for consistency in the names of polynuclear oxoacids, the numerical infix ‘di’ has been uniformly used in naming dinuclear ‘hypo’ acids). Although the ‘meta’ acids are for general nomenclature only, they are preselected names if the structure is unknown.

For consistency in the names of polynuclear oxoacids, the numerical infix ‘di’ has been uniformly used in naming dinuclear ‘hypo’ acids, for example, hypodiphosphorous acid, rather than hypophosphorous acid.

$(HO)_2B\text{-}O\text{-}B(OH)_2$
diboric acid (preselected name)

$(HO)_2B\text{-}B(OH)_2$
hypodiboric acid (preselected name)

$(HO)_3Si\text{-}O\text{-}Si(OH)_3$
disilicic acid (preselected name)

(HO)HP(O)-O-HP(O)(OH)
diphosphonic acid (preselected name)

(HO)(O)HP-PH(O)(OH)
hypodiphosphonic acid (preselected name)

HO-PH-O-PH-OH
diphosphonous acid (preselected name)

(HO)HP-PH(OH)
hypodiphosphonous acid (preselected name)

$(HO)_2P(O)\text{-}O\text{-}P(O)(OH)_2$
diphosphoric acid (preselected name)

$(HO)_2(O)P\text{-}P(O)(OH)_2$
hypodiphosphoric acid (preselected name)

$(HO)_2P\text{-}O\text{-}P(OH)_2$
diphosphorous acid (preselected name)

$(HO)_2P\text{-}P(OH)_2$
hypodiphosphorous acid (preselected name)

(HO)HAs(O)-O-HAs(O)(OH)
diarsonic acid (preselected name)

(HO)(O)HAs-HAs(O)(OH)
hypodiarsonic acid (preselected name)

HO-AsH-O-AsH-OH
diarsonous acid (preselected name)

(HO)HAs-AsH(OH)
hypodiarsonous acid (preselected name)

$(HO)_2As(O)\text{-}O\text{-}As(O)(OH)_2$
diarsoric acid (preselected name)
diarsenic acid

$(HO)_2(O)As\text{-}As(O)(OH)_2$
hypodiarsoric acid (preselected name)
hypodiarsenic acid

$(HO)_2As\text{-}O\text{-}As(OH)_2$
diarsorous acid (preselected name)
diarsenous acid

$(HO)_2As\text{-}As(OH)_2$
hypodiarsorous acid (preselected name)
hypodiarsenous acid

$(HO)HSb(O)\text{-}O\text{-}HSb(O)(OH)$
distibonic acid (preselected name)

$(HO)(O)HSb\text{-}HSb(O)(OH)$
hypodistibonic acid (preselected name)

$HO\text{-}SbH\text{-}O\text{-}SbH\text{-}OH$
distibonous acid (preselected name)

$(HO)HSb\text{-}SbH(OH)$
hypodistibonous acid (preselected name)

$(HO)_2Sb(O)\text{-}O\text{-}Sb(O)(OH)_2$
distiboric acid (preselected name)

$(HO)_2(O)Sb\text{-}Sb(O)(OH)_2$
hypodistiboric acid (preselected name)

$(HO)_2Sb\text{-}O\text{-}Sb(OH)_2$
distiborous acid (preselected name)

$(HO)_2Sb\text{-}Sb(OH)_2$
hypodistiborous acid (preselected name)

$HO\text{-}SO_2\text{-}O\text{-}SO_2\text{-}OH$
disulfuric acid (preselected name)

$HO\text{-}SO_2\text{-}SO_2\text{-}OH$
dithionic acid (preselected name)
hypodisulfuric acid

$HO\text{-}SO\text{-}SO\text{-}OH$
dithionous acid (preselected name)
hypodisulfurous acid

$[HAsO_3]_n = (\text{-}As(O)(OH)O\text{-})_n$
metaarsoric acid
(only for general nomenclature)
metaarsenic acid

$[HAsO_2]_n = (\text{-}As(OH)O\text{-})_n$
metaarsorous acid
(only for general nomenclature)
metaarsenous aicd

$[HBO]_n = (\text{-}B(OH)O\text{-})_n$
metaboric acid
(only for general nomenclature)

$[HPO_3]_n = (\text{-}P(O)(OH)O\text{-})_n$
metaphosphoric acid
(only for general nomenclature)

$[HPO_2]_n = (\text{-}P(OH)O\text{-})_n$
metaphosphorous acid
(only for general nomenclature)

$[H_2SiO_3]_n = (\text{-}Si(OH)_2O\text{-})_n$
metasilicic acid
(only for general nomenclature)

$[HSbO_3]_n = (\text{-}Sb(O)(OH)O\text{-})_n$
metastiboric acid
(only for general nomenclature)

$[HSbO_2]_n$ = $(\text{-}Sb(OH)O\text{-})_n$
metastiborous acid
(only for general nomenclature)

$(HO)HP(O)\text{-}O\text{-}HP(O)\text{-}O\text{-}HP(O)(OH)$
triphosphonic acid (preselected name)

$(HO)_2P(O)\text{-}O\text{-}P(O)(OH)\text{-}O\text{-}P(O)(OH)_2$
triphosphoric acid (preselected name)

$HO\text{-}SO_2\text{-}O\text{-}SO_2\text{-}O\text{-}SO_2\text{-}OH$
trisulfuric acid (preselected name)

P-67.2.2 Functional replacement derivatives of di- and polynuclear noncarbon oxoacids

P-67.2.2.1 General methodology
P-67.2.2.2 Replacement by –OO–, –S–, =S, –Se–, =Se, –Te–, =Te, –NH–, and =NH

P-67.2.2.1 General methodology

Prefixes are used to indicate functional replacement of polynuclear noncarbon oxoacids, listed in P-67.1.2.3.3 and P-67.1.2.3.4. The prefixes are cited and numbered in alphabetical order in front of the retained name of the polyacid, with appropriate locants as required. Each acid is numbered from one end to the other, starting from and finishing at a central atom. Before applying the functional replacement operation, the principal function must be selected; it receives the lower locant. The order of functions to be considered is: acids (see P-67.2.2.2), acid halides and pseudohalides (see P-67.2.3), amides and hydrazides (see P-67.2.4).

P-67.2.2.2 Replacement by –OO–, –S–, =S, –Se–, =Se, –Te–, =Te, –NH–, and =NH

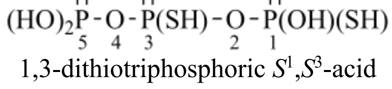
Functional replacement of oxygen atom(s) is denoted by prefixes, i.e., peroxy, for –OO–; thio, for –S– or =S; seleno, for –Se– or =Se; telluro, for –Te– or =Te; and imido, for –NH– or =NH. Superscripted italic letter locants N^1 N^2 are used to designate substitution on imido groups that are not linkages between atoms that receive numerical locants as part of the chain. For rules on primes, see P-16.9.

The use of superscripted ‘*N*’ locants is a change from previous recommendations serially letters for example, ‘N'’, ‘N''’, etc. ; the priming serially follows the arabic numbers of the chain, the number of primes parallels the increasing value of the arabic numbers.

Superscripted italic letters are used to specifically locate the chalcogen atoms in acid groups, for example S^3.

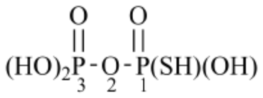
This is a change from previous recommendations where the specific location of a chalcogen atom in acid groups was described by an on line arabic number prefixed to the atomic symbol.

Examples:



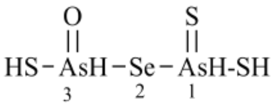
$$(\mathrm{HO})_2\underset{5}{\overset{\mathrm{O}}{\overset{\|}{\mathrm{P}}}}\text{-}\underset{4}{\mathrm{O}}\text{-}\underset{3}{\overset{\mathrm{O}}{\overset{\|}{\mathrm{P}}}}(\mathrm{SH})\text{-}\underset{2}{\mathrm{O}}\text{-}\underset{1}{\overset{\mathrm{O}}{\overset{\|}{\mathrm{P}}}}(\mathrm{OH})(\mathrm{SH})$$

1,3-dithiotriphosphoric S^1,S^3-acid
(not 1,3-dithiotriphosphoric 1-*S*,3-*S*-acid)
(name derived from the preselected name triphosphoric acid)



$$(\mathrm{HO})_2\underset{3}{\overset{\mathrm{O}}{\overset{\|}{\mathrm{P}}}}\text{-}\underset{2}{\mathrm{O}}\text{-}\underset{1}{\overset{\mathrm{O}}{\overset{\|}{\mathrm{P}}}}(\mathrm{SH})(\mathrm{OH})$$

1-thiodiphosphoric S^1-acid (name derived from the preselected name diphosphoric acid;
the ‘thio’ replacement determines locant ‘1’)

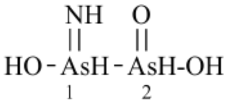


$$\mathrm{HS}\text{-}\underset{3}{\overset{\mathrm{O}}{\overset{\|}{\mathrm{AsH}}}}\text{-}\underset{2}{\mathrm{Se}}\text{-}\underset{1}{\overset{\mathrm{S}}{\overset{\|}{\mathrm{AsH}}}}\text{-SH}$$

2-seleno-1,1,3-trithiodiarsonic S^1,S^3-acid
(name derived from the preselected name diarsonic acid;
the ‘dithio’ replacement for one acid group determines the locant ‘1’)

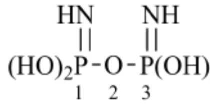
$\mathrm{HS-}\overset{3}{\mathrm{P}}\mathrm{H(O)-}\overset{2}{\mathrm{O}}\mathrm{-}\overset{1}{\mathrm{P}}\mathrm{H(S)-OH}$

1,3-dithiodiphosphonic O^1,S^3-acid
(name derived from the preselected name diphosphonic acid;
the ‘OH’ group of the acid function is alphabetically preferred for lower locant to the ‘SH’ group)



$\mathrm{HO-}\underset{1}{\overset{\mathrm{NH}}{\overset{||}{\mathrm{AsH}}}}\mathrm{-}\underset{2}{\overset{\mathrm{O}}{\overset{||}{\mathrm{AsH}}}}\mathrm{-OH}$

1-imidohypodiarsonic acid
(name derived from the preselected name hypodiarsonic acid;
the ‘imido’ replacement prefix determines the locant ‘1’)



$\mathrm{(HO)_2}\underset{1}{\overset{\mathrm{HN}}{\overset{||}{\mathrm{P}}}}\mathrm{-}\underset{2}{\mathrm{O}}\mathrm{-}\underset{3}{\overset{\mathrm{NH}}{\overset{||}{\mathrm{P}}}}\mathrm{(OH)_2}$

1,3-diimidodiphosphoric acid
(name derived from the preselected name diphosphoric acid)

$\mathrm{HO-}\overset{3}{\mathrm{S}}\mathrm{O_2-}\overset{2}{\mathrm{O}}\mathrm{-}\overset{1}{\mathrm{S}}\mathrm{O_2-SH}$

1-thiodisulfuric S^1-acid
(name derived from preselected name disulfuric acid)

$\mathrm{H_2N-}\overset{3}{\mathrm{S}}\mathrm{O_2-}\overset{2}{\mathrm{O}}\mathrm{-}\overset{1}{\mathrm{S}}\mathrm{O_2-SeH}$

3-amido-1-selenodisulfuric Se^1-acid
(name derived from the preselected name disulfuric acid;
the acid determines the locant ‘1’)

$\mathrm{HO-}\overset{3}{\mathrm{S}}\mathrm{O_2-}\overset{2}{\mathrm{S}}\mathrm{-}\overset{1}{\mathrm{S}}\mathrm{O_2-OH}$

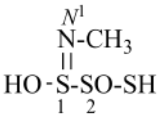
2-thiodisulfuric acid (preselected name)
sulfanedisulfonic acid
trithionic acid (traditional name)

$\mathrm{HO-}\overset{3}{\mathrm{S}}\mathrm{O_2-}\overset{2}{\mathrm{S}}\mathrm{-S-}\overset{1}{\mathrm{S}}\mathrm{O_2-OH}$

2-(dithioperoxy)disulfuric acid (preselected name)
disulfanedisulfonic acid
tetrathionic acid (traditional name)

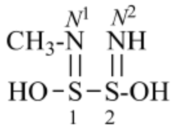
$\mathrm{HO-}\overset{1}{\mathrm{S}}\mathrm{O_2-}\overset{2}{\mathrm{N}}\mathrm{H-}\overset{3}{\mathrm{S}}\mathrm{O_2-}\overset{4}{\mathrm{N}}\mathrm{H-}\overset{5}{\mathrm{S}}\mathrm{O_2-OH}$

2,4-diimidotrisulfuric acid
(name derived from the preselected name trisulfuric acid)



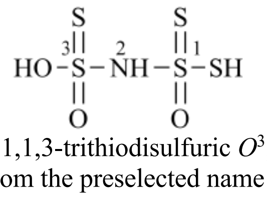
$\mathrm{HO-}\underset{1}{\overset{\overset{N^1}{\mathrm{N-CH_3}}}{\overset{||}{\mathrm{S}}}}\mathrm{-}\underset{2}{\mathrm{SO}}\mathrm{-SH}$

N^1-methyl-1-imido-2-thiodithionous S^2-acid (PIN;
the ‘imido’ replacememt prefix determines the locant ‘1’
[not 1-(methylimido)-2-thiodithionous 2-*S*-acid]



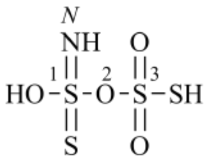
$\mathrm{HO-}\underset{1}{\overset{\overset{N^1}{\mathrm{CH_3-N}}}{\overset{||}{\mathrm{S}}}}\mathrm{-}\underset{2}{\overset{\overset{N^2}{\mathrm{NH}}}{\overset{||}{\mathrm{S}}}}\mathrm{-OH}$

N^1-methyl-1,2-diimidodithionous acid (PIN)



$\mathrm{HO-}{}^{3}\underset{\underset{\mathrm{O}}{||}}{\overset{\mathrm{S}}{\overset{||}{\mathrm{S}}}}\mathrm{-}\overset{2}{\mathrm{NH}}\mathrm{-}\underset{\underset{\mathrm{O}}{||}}{\overset{\mathrm{S}}{\overset{||}{\mathrm{S}}}}{}^{1}\mathrm{-SH}$

2-imido-1,1,3-trithiodisulfuric O^3,S^1-acid
(name derived from the preselected name disulfuric acid)



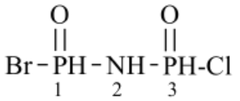
$$\mathrm{HO{-}\overset{NH}{\underset{S}{S}}{-}O{-}\overset{O}{\underset{O}{S}}{-}SH}$$

1-imido-1,3-dithiodisulfuric O^1,S^3-acid
(name derived from the preselected name disulfuric acid;
the ‘OH’ group of the acid function is alphabetically preferred for lower locant to the ‘SH’ group)

P-67.2.3 Acid halides and pseudohalides of di- and polynuclear noncarbon oxoacids

Acid halides and pseudohalides, in which all OH groups have been replaced by halides or pseudohalide atoms or groups, are named by functional class nomenclature by replacing the name ‘acid’ by the name of the appropriate halide or pseudohalide. For acid halides and acid pseudohalides the senority is halides (alphabetical) followed by the following seniority for the halogenides: N_3, CN, NC, NCO, NCS, NCSe, NCTe.

Examples:



$$\mathrm{Br{-}\underset{1}{\overset{O}{PH}}{-}\underset{2}{NH}{-}\underset{3}{\overset{O}{PH}}{-}Cl}$$

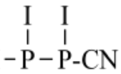
2-imidodiphosphonic 1-bromide 3-chloride
(name derived from the preselected name diphosphonic acid;
the ‘Br’, bromide, is preferred to ‘Cl’, chloride (alphabetically) and determines the locant ‘1’)

$$\mathrm{Cl_2\overset{1}{P}(O){-}\overset{2}{S}{-}\overset{3}{P}(O)Cl_2}$$

2-thiodiphosphoric tetrachloride
(name derived from the preselected name diphosphoric acid)

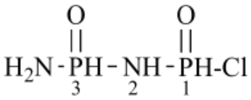
$$\mathrm{(OCN)_2\overset{1}{P}(O){-}\overset{2}{O}{-}\overset{3}{P}(O)(NCO)_2}$$

diphosphoric tetraisocyanate (PIN)



$$\mathrm{I{-}\overset{I}{P}{-}\overset{I}{P}{-}CN}$$

cyanohypodiphosphorous triiodide (PIN)



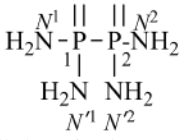
$$\mathrm{H_2N{-}\underset{3}{\overset{O}{PH}}{-}\underset{2}{NH}{-}\underset{1}{\overset{O}{PH}}{-}Cl}$$

3-amido-2-imidodiphosphonic chloride
(name derived from the preselected name diphosphonic acid,
the acid chloride is preferred to the amide group and determines the locant ‘1’)

P-67.2.4 Amides and hydrazides of di- and polynuclear noncarbon oxoacids

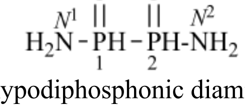
Polynuclear noncarbon oxoacids in which all –OH groups have been replaced by $-NH_2$ or $-NHNH_2$ groups are named as amides or hydrazides, respectively, by functional class nomenclature. Amides are expressed by the class name ‘amide’, preceded by an appropriate multiplying prefix, ‘di’, ‘tri’, etc. Similarly, hydrazides are expressed by the class name ‘hydrazide’. Functional replacement is described by prefixes cited before the whole name and not in front of the class name. Italic letter locants *N*, *N*′, etc. and superscripted letter locants N^1, N'^1, etc. are used to designate substitution on nitrogen atoms that are not linkages between central atoms that receive numerical locants as part of the chain. When a choice is needed, amides are senior to hydrazides, and receive the lower locants.

Examples:



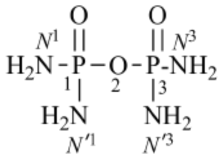
$$\mathrm{\overset{N^1}{H_2N}{-}\overset{O}{\underset{H_2N\,(N'^1)}{\overset{1}{P}}}{-}\overset{O}{\underset{NH_2\,(N'^2)}{\overset{2}{P}}}{-}\overset{N^2}{NH_2}}$$

hypodiphosphoric tetraamide
(name derived from the preselected name hypodiphosphoric acid)



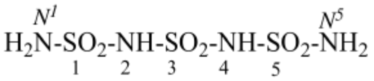
$$\mathrm{\overset{N^1}{H_2N}{-}\underset{1}{\overset{O}{PH}}{-}\underset{2}{\overset{O}{PH}}{-}\overset{N^2}{NH_2}}$$

hypodiphosphonic diamide
(name derived from the preselected name hypodiphosphonic acid)



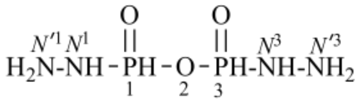
$H_2N\text{-}P(O)(NH_2)\text{-}O\text{-}P(O)(NH_2)\text{-}NH_2$

diphosphoric tetraamide
(name derived from the preselected name diphosphoric acid)



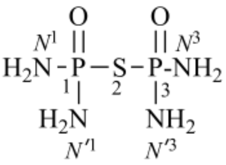
$H_2N\text{-}SO_2\text{-}NH\text{-}SO_2\text{-}NH\text{-}SO_2\text{-}NH_2$

2,4-diimidotrisulfuric diamide
(name derived from the preselected name trisulfuric acid)



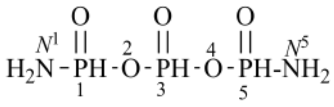
$H_2N\text{-}NH\text{-}PH(O)\text{-}O\text{-}PH(O)\text{-}NH\text{-}NH_2$

diphosphonic dihydrazide
(name derived from the preselected name diphosphonic acid)



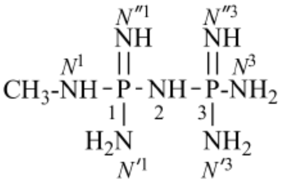
$H_2N\text{-}P(O)(NH_2)\text{-}S\text{-}P(O)(NH_2)\text{-}NH_2$

2-thiodiphosphoric tetraamide
(name derived from the preselected name diphosphoric acid)



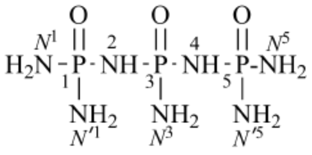
$H_2N\text{-}PH(O)\text{-}O\text{-}PH(O)\text{-}O\text{-}PH(O)\text{-}NH_2$

triphosphonic diamide
(name derived from the preselected name triphosphonic acid)



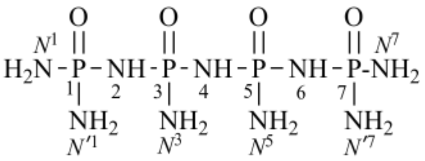
$CH_3\text{-}NH\text{-}P(=NH)(NH_2)\text{-}NH\text{-}P(=NH)(NH_2)\text{-}NH_2$

N^1-methyl-1,2,3-triimidodiphosphoric tetraamide (PIN)



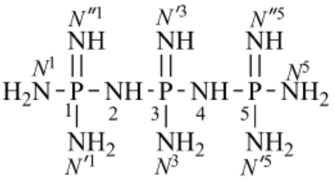
$H_2N\text{-}P(O)(NH_2)\text{-}NH\text{-}P(O)(NH_2)\text{-}NH\text{-}P(O)(NH_2)\text{-}NH_2$

2,4-diimidotriphosphoric pentaamide
(name derived from the preselected name triphosphoric acid)



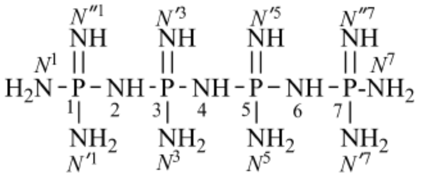
$H_2N\text{-}P(O)(NH_2)\text{-}NH\text{-}P(O)(NH_2)\text{-}NH\text{-}P(O)(NH_2)\text{-}NH\text{-}P(O)(NH_2)\text{-}NH_2$

2,4,6-triimidotetraphosphoric hexaamide
(name derived from the preselected name tetraphosphoric acid)



$H_2N\text{-}P(=NH)(NH_2)\text{-}NH\text{-}P(=NH)(NH_2)\text{-}NH\text{-}P(=NH)(NH_2)\text{-}NH_2$

pentaimidotriphosphoric pentaamide
(name derived from the preselected name triphosphoric acid)



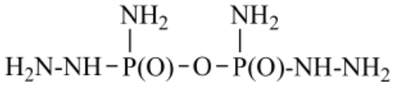
$$\overset{N^1}{H_2N}-\overset{N''^1}{\overset{NH}{\overset{\|}{\underset{\underset{N'^1}{NH_2}}{\underset{|}{\underset{1}{P}}}}}}-\underset{2}{NH}-\overset{N'^3}{\overset{NH}{\overset{\|}{\underset{\underset{N^3}{NH_2}}{\underset{|}{\underset{3}{P}}}}}}-\underset{4}{NH}-\overset{N'^5}{\overset{NH}{\overset{\|}{\underset{\underset{N^5}{NH_2}}{\underset{|}{\underset{5}{P}}}}}}-\underset{6}{NH}-\overset{N''^7}{\overset{NH}{\overset{\|}{\underset{\underset{N'^7}{NH_2}}{\underset{|}{\underset{7}{P}}}}}}-\overset{N^7}{NH_2}$$

heptaimidotetraphosphoric hexaamide
(name derived from the preselected name tetraphosphoric acid)

$H_2N-SO_2-O-SO_2-NH_2$
disulfuric diamide
(name derived from the preselected name disulfuric acid)

$H_2N-SeO_2-O-SeO_2-NH_2$
diselenic diamide
(name derived from the preselected name diselenic acid)

$H_2N-\overset{1}{P}H(O)-\overset{2}{O}-\overset{3}{P}H(O)-NH-NH_2$
3-hydrazidodiphosphonic 1-amide



$$H_2N-NH-\overset{NH_2}{\overset{|}{P}}(O)-O-\overset{NH_2}{\overset{|}{P}}(O)-NH-NH_2$$

1,3-dihydrazidodiphosphoric 1,3-diamide

P-67.2.5 Salts, esters, and anhydrides of di- and polynuclear noncarbon oxoacids

P-67.2.5.1 Salts of di- and polybasic noncarbon oxoacids
P-67.2.5.2 Esters of polybasic noncarbon oxoacids
P-67.2.5.3 Anhydrides of polybasic noncarbon oxoacids

P-67.2.5.1 Salts of di- and polynuclear noncarbon oxoacids

P-67.2.5.1.1 Neutral salts of di- and polynuclear noncarbon oxoacids are named by citing the cation(s) followed by the name of the anion(s) as (a) separate word(s). Names of anions are formed by changing the ‘ic acid’ ending to ‘ate’ and the ‘ous acid’ to ‘ite’. Different cations are cited in alphabetical order.

Examples:

$2\ Na^+\quad {}^-O-\underset{1}{S}(=\overset{N^1}{N}-CH_3)-\underset{2}{S}(=NH)-O^-$
disodium *N*-methyl-1,2-diimidodithionite (PIN)

$4\ Na^+\quad ({}^-O)_2P(=O)-O-P(=O)(O^-)_2$
tetrasodium diphosphate
(name derived from the preselected name diphosphoric acid)

P-67.2.5.1.2 Acid salts of di- and polynuclear noncarbon oxoacids are named in the same way as neutral salts, the remaining acid hydrogen atom(s) being indicated by the word ‘hydrogen’ (or ‘dihydrogen’, etc., as appropriate) inserted between the name of the cation and the name of the anion from which it is separated by spaces.

Example:

$NaO-SO_2-SS-SO_2-OH$
sodium hydrogen 2-dithioperoxydisulfate
(name derived from the preselected name disulfuric acid)

P-67.2.5.2 Esters of polynuclear noncarbon oxoacids

Fully esterified polynuclear noncarbon oxoacids are named as neutral salts, except that names of allowed groups (alkyl groups, aryl groups, etc.), cited in alphanumerical order when more than one, replace the name of the cations. Partial (acid) esters of polybasic noncarbon oxoacids and their salts are named by the procedures for neutral esters and acid salts, except that the name ‘hydrogen’ denoting acid hydrogen atoms is indicated by the separate word ‘hydrogen’ (with the appropriate multiplying prefix denoting multiplicity) inserted between the name of the cation or of the organic group and the name of the anion.

Examples:

$CH_3\text{-}S\text{-}\overset{1}{P}H\text{-}\overset{2}{P}H\text{-}O\text{-}CH_3$
dimethyl thiohypodiphosphonite (PIN)

$HS\text{-}\overset{1}{P}H\text{-}\overset{2}{P}H\text{-}S\text{-}CH_3$
methyl hydrogen dithiohypodiphosphonite (PIN)

$CH_3\text{-}O\text{-}SO_2\text{-}O\text{-}SO_2\text{-}S\text{-}CH_2\text{-}CH_3$
S-ethyl *O*-methyl thiodisulfate (PIN)

$(CH_3)_2CH\text{-}O\text{-}SO\text{-}O\text{-}SO\text{-}O\text{-}CH(CH_3)_2$
1,3-bis[(propan-2-yl)oxy]-$1\lambda^4,3\lambda^4$-dithioxane-1,3-dione (PIN)
[not di(propan-2-yl) disulfite, see P-67.3.2]

$CH_3\text{-}O\text{-}SO_2\text{-}S\text{-}SO_2\text{-}O\text{-}CH_3$
O^1,O^3-dimethyl thiodisulfate (PIN)

P-67.2.5.3 Anhydrides of polynuclear non-carbon oxoacids

Neutral anhydrides formed between organic acids and polynuclear noncarbon oxoacids having preselected names are named by citing, in alphabetical order, the names of the acids followed by the name of the class ‘anhydride’; multiplying prefixes ‘di’, ‘tri’, etc. are used to indicate the multiplicity of the anhydride linkages.

Acidic anhydrides are named by using the senior acid as parent or by using systematic substitutive nomenclature as described in P-67.3.1.

Examples:

$(CH_3\text{-}CO\text{-}O)_2P(O)\text{-}P(O)(O\text{-}CO\text{-}CH_3)_2$
tetraacetic hypodiphosphoric tetraanhydride (PIN)

$CH_3\text{-}CO\text{-}O\text{-}SO\text{-}SO\text{-}O\text{-}CO\text{-}CH_2\text{-}CH_3$
acetic dithionous propanoic dianhydride (PIN)
acetic hypodisulfurous propanoic dianhydride

P-67.2.6 Substituent groups derived from polyacids

In the presence of a characteristic group having precedence for citation as principal group, polynuclear noncarbon oxoacids are cited as prefixes. The names of these prefixes are formed by:

(1) combinations of acyl groups;

(2) on the basis of the names of the group which includes the greatest number of P, As, Sb, S, Se, and Te central atoms.

(3) skeletal replacement nomenclature (see P-15.4 and P-51.4), when conditions for its use are satisfied.

When there is a choice for parent substituent, seniority is given to parent substituents having the largest size, then, if needed, to alphanumerical order.

Examples:

$(HO)_2P(O)\text{-}O\text{-}P(O)(OH)\text{-}O\text{-}\overset{3}{C}H_2\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}OOH$
(2) 3-[(1,3,3-trihydroxy-1,3-dioxo-$1\lambda^5,3\lambda^5$-diphosphoxan-1-yl)oxy]propanoic acid (PIN)
(1) 3-{[hydroxy(phosphonooxy)phosphoryl]oxy}propanoic acid

$\overset{1}{C}H_3\text{-}\overset{2}{O}\text{-}\overset{3}{S}(O)\text{-}\overset{4}{O}\text{-}\overset{5}{S}(O)\text{-}\overset{6}{O}\text{-}\overset{7}{S}(O)\text{-}\overset{8}{O}\text{-}\overset{9}{C}H_2\text{-}\overset{10}{C}OOH$
(3) 3,5,7-trioxo-2,4,6,8-tetraoxa-$3\lambda^4,5\lambda^4,7\lambda^4$-trithiadecan-10-oic acid (PIN)
(1) {[({[(methoxysulfinyl)oxy]sulfinyl}oxy)sulfinyl]oxy}acetic acid
(2) [(5-methoxy-1,3,5-trioxo-$1\lambda^4,3\lambda^4,5\lambda^4$-trisulfoxan-1-yl)oxy]acetic acid

$\overset{1}{C}H_3\text{-}\overset{2}{S}\text{-}\overset{3}{S}(S)\text{-}\overset{4}{S}\text{-}\overset{5}{S}(S)\text{-}\overset{6}{S}\text{-}\overset{7}{C}H_2\text{-}\overset{8}{C}H_2\text{-}\overset{9}{C}OOH$
(3) 3,5-bis(sulfanylidene)-$2,3\lambda^4,4,5\lambda^4$,6-pentathianonan-9-oic acid (PIN)
(2) 3-[5-methyl-2,4-bis(sulfanylidene)-$2\lambda^4,4\lambda^4$-pentasulfanyl]propanoic acid
(1) 3-[({[(methylsulfanyl)sulfinothioyl]sulfanyl}sulfinothioyl)sulfanyl]propanoic acid

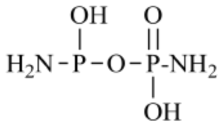
P-67.3 SUBSTITUTIVE NAMES AND FUNCTIONAL CLASS NAMES OF POLYACIDS

P-67.3.1 Names of polynuclear noncarbon oxoacids that cannot be formed on the basis of fundamental oxoacids are either named by using class names, such as anhydrides, or they are formed substitutively. Anhydride names are preferred to substitutive names.

Some names are also included in this Section because their structure does not correspond to the name implied by a diacid or a hypodiacid, for example the name 'disulfurous acid', exemplified below.

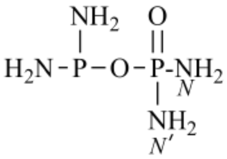
Names of derivatives of acids that cannot be formed directly by functional replacement are generated by substitution of acids with preferred names such as phosphonic acid and phosphinic acid; or they are class names such as 'anhydride'. The parent is chosen in accordance with the seniority order of classes: acids, acid halides, azides, cyanides, isocyanides, isocyanates (and chalcogen analogues in the order O > S > Se > Te), amides, hydrazides, and the maximum number of groups representing the senior class (see P-67.1.2.3.2).

Examples:



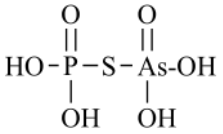
$H_2N-\overset{OH}{P}-O-\overset{O}{\underset{OH}{P}}-NH_2$

{[amino(hydroxy)phosphanyl]oxy}phosphonamidic acid (preselected name)
(phosphonamidic acid is senior to phosphonamidous acid)
phosphoramidic phosphoramidous monoanhydride
(an acid is preferred to an anhydride in the seniority order of classes)



$H_2N-\overset{NH_2}{P}-O-\overset{O}{\underset{\underset{N'}{NH_2}}{P}}-\underset{N}{NH_2}$

phosphorodiamidic phosphorodiamidous anhydride (preselected name)
[(diaminophosphanyl)oxy]phosphonic diamide
(an anhydride is senior to an amide)



$HO-\overset{O}{\underset{OH}{P}}-S-\overset{O}{\underset{OH}{As}}-OH$

(arsonosulfanyl)phosphonic acid (preselected name)
arsoric phosphoric thiomonoanhydride
(an acid is senior to an anhydride; the phosphorus acid is senior to the arsenic acid)

$(HO)HP(O)-\overset{N}{N}H-P(O)(OH)_2$

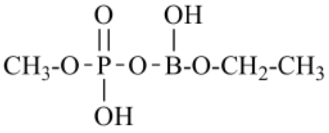
N-(hydroxyphosphonoyl)phosphoramidic acid (preselected name)
(only a substitutive name is possible in this case)

$(HO)_2P-HP(O)-OH$
(dihydroxyphosphanyl)phosphinic acid (preselected name)

$(CH_3-O)_2P(O)-O-HP(O)-O-CH_3$
methyl [(dimethoxyphosphoryl)oxy]phosphonate (PIN)
(phosphonic acid is senior to phosphoric acid; see P-42)
(formerly trimethyl isohypophosphate)

$(CH_3)_2P-P(OH)-P(CH_3)_2$
bis(dimethylphosphanyl)phosphinous acid (PIN)
(not 1,1,3,3-tetramethyltriphosphan-2-ol;
the acid is senior to the heterol)

$HO-\overset{1}{S}I_2-S-CN$
1-hydroxy-1,1-diiodo-1λ^4-disulfane-2-carbonitrile (PIN)
(formerly diiodo(thiocyanatido)orthosulfurous acid)
(not orthosulfurodiiodidothiocyanatidous acid)



$CH_3-O-\overset{O}{\underset{OH}{P}}-O-\overset{OH}{B}-O-CH_2-CH_3$

methyl hydrogen {[ethoxy(hydroxy)boranyl]oxy}phosphonate (PIN)
(ethyl dihydrogen borate) (methyl dihydrogen phosphate) anhydride

CH_3-CO-O-P(O)(OH)$_2$
(acetyloxy)phosphonic acid (PIN)
acetic phosphoric monoanhydride
monoacetyl phosphate

HO-SeO$_2$-O-SO$_2$-OH
selenic sulfuric anhydride (preselected name)
(selenonooxy)hydroxy-λ^6-sulfanedione

CH_3-CH_2-CO-O-B(OH)$_2$
(propanoyloxy)boronic acid (PIN)
boric propanoic monoanhydride

CH_3-CO-O-CO-O-CO-OH
{[(acetyloxy)carbonyl]oxy}formic acid (PIN)
acetic dicarbonic monoanhydride

P-67.3.2 The disulfurous acid name dilemma

The name disulfurous acid should correspond to the structure HO-SO-O-SO-OH implied for all homogeneous diacids in accordance with the definition given in P-67.2. As the reported structure, HO-SO-SO$_2$-OH, is called 'disulfurous acid' in the *Nomenclature of Inorganic Chemistry* (ref. 12) a different name must be assigned to HO-SO-O-SO-OH. A substitutive name is appropriate in this situation.

Since the name 'disulfurous acid' is used for HO-SO-SO$_2$-OH in the Nomenclature of Inorganic Chemistry ref. 12), it cannot be used in the systematic way for HO-SO-O-SO-OH. Accordingly, the preselected name for the latter is '1,3-dihydroxy-1λ^4,3λ^4-dithioxane-1,3-dione'.

Examples:

HO-SO-O-SO-OH
1,3-dihydroxy-1λ^4,3λ^4-dithioxane-1,3-dione (preselected name)

CH_3-O-S(=O)-O-S(=O)-O-CH_3
1,3-dimethoxy-1λ^4,3λ^4-dithioxane-1,3-dione (PIN)

CH_3-O-S(=NH)-O-S(=NH)-O-CH_3
1,3-dimethoxy-1λ^4,3λ^4-dithioxane-1,3-diimine (PIN)

P-68 NOMENCLATURE FOR ORGANIC COMPOUNDS OF THE GROUP 13, 14, 15, 16, AND 17 ELEMENTS NOT INCLUDED IN SECTIONS P-62 THROUGH P-67

P-68.0 Introduction
P-68.1 Nomenclature for compounds of the Group 13 elements
P-68.2 Nomenclature for compounds of the Group 14 elements
P-68.3 Nomenclature for compounds of the Group 15 elements
P-68.4 Nomenclature for compounds of the Group 16 elements
P-68.5 Nomenclature for compounds of the Group 17 elements

P-68.0 INTRODUCTION

The nomenclature of organic compounds is based on two approaches. General principles, rules, and conventions applicable, with some rare exceptions, to all compounds of elements belonging to Groups 13 through 17; they have been described and illustrated in previous Chapters. Another approach is based on the identical treatment of compounds within one Group. Up until now the nomenclature of compounds of Group 13 was compounds of the element boron; these will be included in a future publication by another group. It is advantageous to describe all compounds of a Group in the same manner to identify clearly their similarities and underline exceptions, if any. This method should facilitate naming of new compounds by comparison with established models.

Another aspect of nomenclature that is described Group by Group would be to easily grasp the general patterns of the different Groups. The nomenclature of Group 15 is diverse; suffixes are associated with nitrogen, mononuclear and polynuclear acids are the base of many derivatives of phosphorus, arsenic, and many compounds of antimony and bismuth compounds are named substitutively. By comparison, compounds of Group 14 are essentially named by substitutive nomenclature. Thus, the compound C_6H_5-PH-OCH_3 is named by functional class nomenclature as an ester, i.e., methyl phenylphosphinite, but the compound, C_6H_5-SnH(OCH_3)$_2$ is named substitutively as dimethoxy(phenyl)stannane in spite of their apparent similarity of structures.

There is a third purpose for this Section about Groups 13 through 17. In it, substitutive nomenclature treats metals, semi-metals, and non-metals equally when a compound contains carbon. The Group treatment illustrates many aspects of the nomenclature of organometallic compounds. This is particularly evident for the nomenclature of compounds of the Groups 13 and 14 elements, for which the extensive and well known nomenclature for boron and carbon compounds serves as models to name the other compounds of the Group.

For boron and the metals of Groups 14 and 15, i.e., Ge, Sn, Pb, Sb, and Bi, the same principles are followed as in other sections of these recommendations, namely, if the compound contains carbon and can be named by substitutive nomenclature principles given elsewhere in these recommendations based on acceptable parent hydride names, it is assigned a PIN; however, if there is no carbon present, the name is described as a preselected parent hydride or a name based on a preselected parent hydride or compound. Finally, for many compounds of these elements, their structures are not consistent with the principles of substitutive nomenclature; these, then, are named by the principles of inorganic and coordination nomenclature, for which see ref. 12.

P-68.1 NOMENCLATURE FOR COMPOUNDS OF THE GROUP 13 ELEMENTS

Except for the polynuclear boron hydrides, boron compounds have traditionally been included in the recommendations for naming organic compounds. However, substitutive nomenclature has been applied on the basis of parent hydrides, their substituent groups, and appropriate operations to complement the nomenclature of polynuclear boron compounds, for example names formed by skeletal replacement (‘a’) nomenclature, multiplicative nomenclature, and names derived from the functional parent acids based on boric acid, $B(OH)_3$, boronic acid, $HB(OH)_2$, and borinic acid, $H_2B(OH)$; these are retained functional parent compounds.

The nomenclature of Al, Ga, In, and Tl compounds in these recommendations, including formal organometallic compounds, is patterned on boron nomenclature and is recommended only for use in general nomenclature. Recommendations of preferred IUPAC names for most compounds of these elements will appear in a later publication by another group.

P-68.1.1 Parent hydrides
P-68.1.2 Names for substituent groups derived from parent hydrides
P-68.1.3 Modification of the degree of hydrogenation
P-68.1.4 Functional parent compounds
P-68.1.5 Substitutive nomenclature
P-68.1.6 Adducts

P-68.1.1 Parent hydrides

P-68.1.1.1 Mononuclear hydrides
P-68.1.1.2 Acyclic polynuclear hydrides
P-68.1.1.3 Cyclic hydrides

P-68.1.1.1 Mononuclear hydrides

The names of the mononuclear hydrides are listed in Table 2.1. The standard bonding number is 3 and the λ-convention (see P-14.1) is used to indicate nonstandard bonding numbers. The names of these parent hydrides are all preselected names (see P-12.2).

Examples:

BH_3
borane (preselected name)

BH
λ^1-borane (preselected name)

AlH_3
alumane (preselected name)

GaH_3
gallane (preselected name)

InH_3
indigane (preselected name)

TlH_3
thallane (preselected name)

P-68.1.1.2 Acyclic polynuclear hydrides

P-68.1.1.2.1 Acyclic di- and polynuclear parent hydrides are named by citing the number of skeletal atoms in the molecule as a multiplying prefix, ‘di’, ‘tri’, etc., in front of the name of the mononuclear parent hydride. The number of hydrogen atoms in the molecule is designated by an arabic numeral enclosed in parentheses immediately following the name derived as above. These numbers are omitted when there is no ambiguity or by convention in the names of acyclic polynuclear hydrides. A specific nomenclature is used to name polycyclic polyboranes; these names are described in Chapter IR-6.2.3 of ref. 12. Parent hydrides are preselected names.

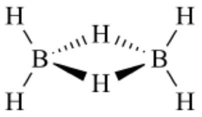
Examples:

$H_2\overset{2}{B}\text{-}\overset{1}{B}H_2$

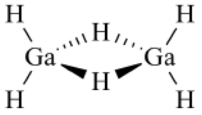
diborane(4) (preselected name)

$H_2\overset{3}{B}\text{-}\overset{2}{B}H\text{-}\overset{1}{B}H_2$

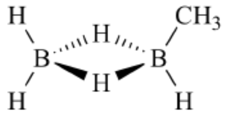
triborane(5) (preselected name)



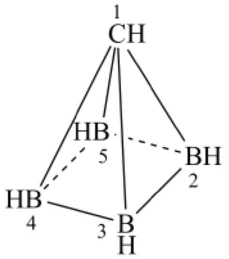
diborane(6) (preselected name)



digallane(6) (preselected name)



1-methyldiborane(6) (PIN)



1-carba-*nido*-pentaborane(5) (PIN)

P-68.1.1.2.2 Compounds formed of alternating heteroatoms are named in accordance with Rule P-21.2.3.1 . They are considered as nonfunctional parent structures having preselected names, except when nitrogen atoms are present; then the compounds are named as amines (see P-62.2.).

> When nitrogen atoms are present, this is a change from the 1993 Guide (ref. 2) because the 'amine' characteristic group was not recognized there.

Examples:

$(CH_3)_2\overset{3}{B}\text{-}\overset{2}{O}\text{-}\overset{1}{B}(CH_3)_2$

tetramethyldiboroxane (PIN)

$H_2\overset{5}{Al}\text{-}\overset{4}{O}\text{-}\overset{3}{Al}H\text{-}\overset{2}{O}\text{-}\overset{1}{Al}H_2$

trialuminoxane (preselected name)

$CH_3\text{-}\overset{1}{B}H\text{-}\overset{N}{N}H\text{-}BH\text{-}CH_3$

1-methyl-*N*-(methylboranyl)boranamine (PIN)

P-68.1.1.2.3 Compounds named by skeletal replacement ('a') nomenclature (see P-15.4)

Examples:

$\overset{10}{C}H_3\text{-}\overset{9}{B}(CH_3)\text{-}\overset{8}{C}H_2\text{-}\overset{7}{O}\text{-}\overset{6}{C}H_2\text{-}\overset{5}{C}H_2\text{-}\overset{4}{O}\text{-}\overset{3}{C}H_2\text{-}\overset{2}{B}(CH_3)\text{-}\overset{1}{C}H_3$

2,9-dimethyl-4,7-dioxa-2,9-diboradecane (PIN)
[ethane-1,2-diylbis(oxymethylene)]bis(dimethylborane)

$H_2\overset{9}{B}\text{-}\overset{8}{C}H_2\text{-}\overset{7}{Si}H_2\text{-}\overset{6}{C}H_2\text{-}\overset{5}{Si}H_2\text{-}\overset{4}{C}H_2\text{-}\overset{3}{Si}H_2\text{-}\overset{2}{C}H_2\text{-}\overset{1}{B}H_2$

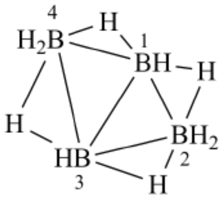
3,5,7-trisila-1,9-diboranonane (PIN)
[silanediylbis(methylene)]bis[(boranylmethyl)silane]
Si,Si′-bis(boranylmethyl)[silanediylbis(methylene)]bis(silane)

P-68.1.1.3 Cyclic parent hydrides

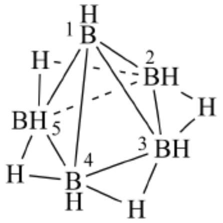
P-68.1.1.3.1 Polyhedral polyboranes.

Nomenclature of polyhedral polyboranes constitute a rich and diversified system characterized by specific prefixes. It has been described and illustrated in the Section IR-6.2.3 (ref. 12); it is not reproduced in these recommendations.

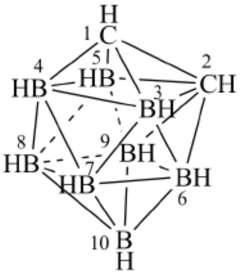
Examples:



arachno-tetraborane(10)
(preselected name)



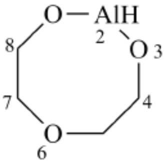
nido-pentaborane(9)
(preselected name)



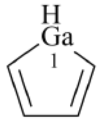
1,2-dicarba-*closo*-decaborane(10) (PIN)

P-68.1.1.3.2 Heterocyclic parent hydrides containing Group 13 atom(s) belong to all the different classes of rings and ring systems described in Chapter P-2. Preferred IUPAC names are selected according to the general rules given for each class.

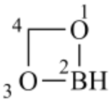
Examples:



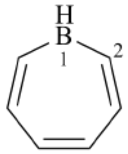
1,3,6,2-trioxaluminocane
(not 1,3,6-trioxa-2-aluminacyclooctane)



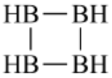
1*H*-gallole
(not 1-gallacyclopenta-2,4-diene)



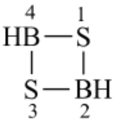
1,3,2-dioxaboretane (PIN)
(not 1,3-dioxa-2-boracyclobutane)



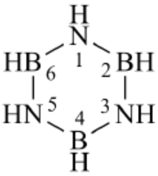
1*H*-borepine (PIN)
(not 1*H*-1-boracyclohepta-2,4,6-triene)



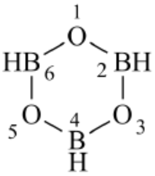
tetraboretane (preselected name; see P-12.2; P-22.2.5)
cyclotetraborane(4)
(not 1,2,3,4-tetraboracyclobutane)



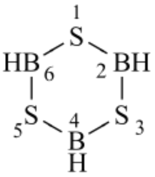
1,3,2,4-dithiadiboretane (preselected name; see P-12.2; P-22.2.6)
cyclodiborathiane
(not 1,3-dithia-2,4-diboracyclobutane)



1,3,5,2,4,6-triazatriborinane
(preselected name)
borazine (see D-7.54, ref. 1)
cyclotriborazane
(not 1,3,5-triaza-2,4,6-triboracyclohexane)



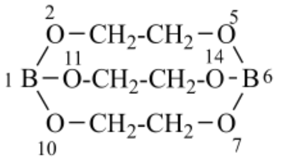
1,3,5,2,4,6-trioxatriborinane (preselected name)
boroxin (see D-7.54, ref. 1)
cyclotriboroxane
(not 1,3,5-trioxa-2,4,6-triboracyclohexane)



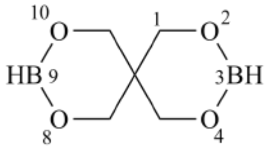
1,3,5,2,4,6-trithiatriborinane (preselected name)
borthiin (see D-7.54, ref. 1)
cyclotriborathiane
(not 1,3,5-trithia-2,4,6-triboracyclohexane)

P-68.1.1.3.3 von Baeyer and spiro compounds (see also P-23 and P-24)

Examples:



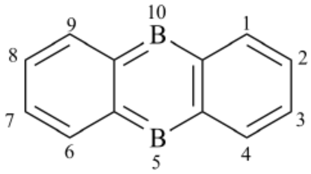
2,5,7,10,11,14-hexaoxa-1,6-diborabicyclo[4.4.4]tetradecane (PIN)



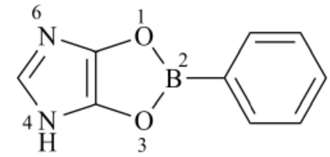
2,4,8,10-tetraoxa-3,9-diboraspiro[5.5]undecane (PIN)

P-68.1.1.3.4 Fused ring systems (see also P-25)

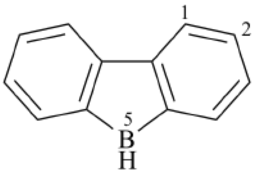
Examples:



boranthrene (PIN)



2-phenyl-2*H*,4*H*-[1,3,2]dioxaborolo[4,5-*d*]imidazole (PIN)



5*H*-dibenzo[*b*,*d*]borole (PIN)

P-68.1.2 Names of substituent groups derived from parent hydrides

Names of substituent groups $-BH_2$ and $=BH$ derived from borane are formed by method (2) described in P-29.2; they are preselected prefixes.

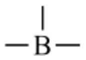
Prefixes derived from borane are no longer named by method (1) in P-29.2.

Examples:

$-BH_2$
boranyl (preselected prefix)
(not boryl)

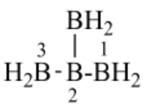
$=BH$
boranylidene (preselected prefix)
(not borylidene)

$>BH$
boranediyl (preselected prefix)
(not borylidene)
(not borylene)



$$-\overset{|}{B}-$$

boranetriyl (preselected prefix)
(not borylidyne)



$$\overset{3}{H_2B}-\underset{2}{\overset{BH_2}{B}}-\overset{1}{BH_2}$$

2-boranyltriborane(5) (preselected prefix)

$$\overset{1}{-BH}-\overset{2}{BH}-\overset{3}{BH_2}$$

triboran(5)-1-yl (preselected prefix)

$-BH-O-BH_2$
diboroxanyl (preselected prefix)

$–BH\text{-}NH\text{-}BH_2$
(boranylamino)boranyl (preselected prefix)
(not diborazan-1-yl)

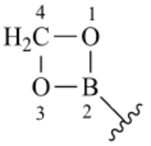
$H_2Al–$
alumanyl
(preselected prefix)

$H_2Ga–$
gallanyl
(preselected prefix)

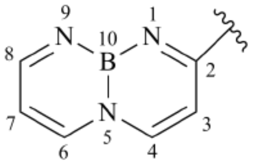
$H_2In–$
indiganyl
(preselected prefix)

$H_2Tl–$
thallanyl
(preselected prefix)

$\overset{1}{CH_3}\text{-}\overset{2}{SiH_2}\text{-}CH_2\text{-}\overset{4}{SiH_2}\text{-}CH_2\text{-}\overset{6}{SiH_2}\text{-}CH_2\text{-}\overset{8}{BH}\text{-}\overset{9}{CH_2}–$
2,4,6-trisila-8-boranonan-9-yl (preferred prefix)



1,3,2-dioxaboretan-2-yl (preferred prefix)



[1,3,2]diazaborinino[1,2-*a*][1,3,2]diazaborinin-2-yl (preferred prefix)

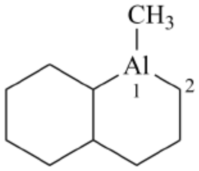
P-68.1.3 Modification of the degree of hydrogenation

Double bonds are denoted by the ‘ene’ ending or by saturation of double bonds of mancude ring systems by the use of ‘hydro’ prefixes, as described in Sections P-31.1 and P-31.2, respectively.

Hydro/dehydro prefixes are now classified as detachable prefixes but are not included in the category of alphabetized detachable prefixes (see P-14.4; see also P-15.1.5.2, P-31.2, P-58.2).

Examples:

$H\overset{1}{B}{=}\overset{2}{B}\text{-}\overset{3}{B}H_2$
triborene(5) (preselected name)



1-methyldecahydro-1-benzaluminine

P-68.1.4 Functional parent compounds

P-68.1.4.1 The names boric acid, boronic acid, and borinic acid are preselected retained names for the compounds $B(OH)_3$, $HB(OH)_2$, and $H_2B(OH)$, respectively (see P-67.1.1). They are preferred IUPAC names for deriving the names of the corresponding salts, esters, or anhydrides; or when the hydrogen atom(s) attached to the boron atom is (are) substituted, for example methylboronic acid for $CH_3\text{-}B(OH)_2$. Chalcogen analogues are named using infixes to denote functional replacement of oxygen by S, Se, and Te.

Acid names such as these are not used for other elements of Group 13, which are named using substitutive nomenclature based on the appropriate parent hydride. For names such as methaneboronic acid vs. methylboronic acid for $CH_3\text{-}B(OH)_2$, see P-67.1.1.2.

Examples:

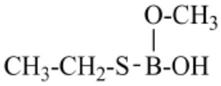
$CH_3\text{-}B(O^-)_2\ 2\ Na^+$
disodium methylboronate (PIN)

$CH_3\text{-}B(O^-)(OH)\ Na^+$
sodium hydrogen methylboronate (PIN)

$CH_3\text{-}B(OH)_2$
methylboronic acid (PIN)
(not methylboranediol)

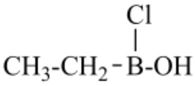
$(CH_3)_2B(SH)$
dimethylborinothioic acid (PIN)
dimethyl(thioborinic) acid
(not dimethylboranethiol)

$B(S\text{-}CH_3)_3$
trimethyl borotrithioate (PIN)
trimethyl trithioborate



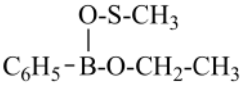
$$CH_3\text{-}CH_2\text{-}S\text{-}\overset{\overset{\displaystyle O\text{-}CH_3}{|}}{B}\text{-}OH$$

S-ethyl *O*-methyl hydrogen borothioate (PIN)
S-ethyl *O*-methyl hydrogen thioborate



$$CH_3\text{-}CH_2\text{-}\overset{\overset{\displaystyle Cl}{|}}{B}\text{-}OH$$

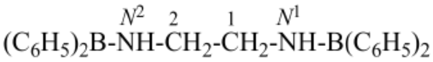
ethylboronochloridic acid (PIN)
ethylchloroboronic acid; chloro replaces an OH group of boronic acid)
chloro(ethyl)borinic acid
(chloro and ethyl substitute the H atoms of borinic acid)



$$C_6H_5\text{-}\overset{\overset{\displaystyle O\text{-}S\text{-}CH_3}{|}}{B}\text{-}O\text{-}CH_2\text{-}CH_3$$

O-ethyl *OS*-methyl phenylborono(thioperoxoate) (PIN)
O-ethyl *OS*-methyl phenyl(thioperoxy)boronate

$(CH_3)_2Al\text{-}O^-\ Na^+$
sodium dimethylalumanolate



$$(C_6H_5)_2B\text{-}\overset{N^2}{NH}\text{-}\overset{2}{CH_2}\text{-}\overset{1}{CH_2}\text{-}\overset{N^1}{NH}\text{-}B(C_6H_5)_2$$

N^1,N^2-bis(diphenylboranyl)ethane-1,2-diamine (PIN)
[not *N*,*N*′-(ethane-1,2-diyl)bis(diphenylborinic amide);
not *N*,*N*′-(ethane-1,2-diyl)bis(diphenylboranamine);
not 1,1,6,6-tetraphenyl-2,5-diaza-1,6-diborahexane]

P-68.1.4.2 Substituent groups for the boron acids

The general methodology for forming substituent groups derived from the boron acids has been described in P-67.1.4.2. Except for the name ‘borono’ for $(HO)_2B$– which is retained, their names are formed substitutively based on the parent hydride ‘borane’, BH_3. Chalcogen analogues of ‘borono’ are named by replacement prefixes, and not replacement infixes.

Examples:

$(HO)_2B$–
borono (preselected prefix)
dihydroxyboranyl

$(HS)BH$–
sulfanylboranyl (preselected prefix)

$(HO)(HS)B$–
thioborono (preselected prefix)
hydroxy(sulfanyl)boranyl

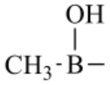
$(HSe)_2B$–
diselenoborono (preselected prefix)
bis(selanyl)boranyl

Cl-BH–
chloroboranyl (preselected prefix)
(not chloroboryl)

$(H_2N)_2B$–
diaminoboranyl (preselected prefix)

$(CH_3)_2B$-O–
(dimethylboranyl)oxy (preferred prefix)

CH_3-BH-NH–
(methylboranyl)amino (preferred prefix)



CH_3-B(OH)–

hydroxy(methyl)boranyl (preferred prefix)

P-68.1.5 Substitutive nomenclature

Derivatives of borane, BH_3, are named by substitutive nomenclature, the substituents being denoted by suffixes and prefixes in accordance with the principles, rules, and conventions of substitutive nomenclature. The three acids described in P-68.1.4 have retained names that are preselected names.

Derivatives are named in accordance with the seniority of classes described by the general rule in Section P-41. Thus, acids having retained names have seniority over other suffixes. Suffixes are used when recommended in substitutive nomenclature, in accordance with the general rule described in Section P-43. In the absence of a suffix that has priority for naming organic compounds, when a choice is possible for selecting the parent hydride, the seniority order is as follows: N > P > As > Sb > Bi > Si > Ge > Sn > Pb > B > Al > Ga > In > Tl > O > S > Se > Te > C (substituent groups).

P-68.1.5.1 Suffix nomenclature
P-68.1.5.2 Prefix nomenclature

P-68.1.5.1 Suffix nomenclature

Suffixes, when available, are used to denote characteristic groups; prefixes are not recommended. Suffixes containing a carbon atom generate preferred IUPAC names.

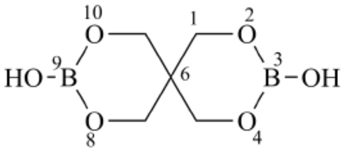
Examples:

H_2B-CN
boranecarbonitrile (PIN)

$(HO)_2B$-$B(OH)_2$
hypodiboric acid (preselected name; see P-67.2.1)
diborane(4)tetrol
[not tetrahydroxydiborane(4)]

$(CH_3)_2Tl$-OH
dimethylthallanol
hydroxydi(methyl)thallane

$(CH_3)_2Tl$-O^- Na^+
sodium dimethylthallanolate



2,4,8,10-tetraoxa-3,9-diboraspiro[5.5]undecane-3,9-diol (PIN)

P-68.1.5.2 Prefix nomenclature

P-68.1.5.2.1 Substituted parent hydrides
P-68.1.5.2.2 Compounds with bridging atoms or groups
P-68.1.5.2.3 Compounds with groups of higher seniority

P-68.1.5.2.1 Substituted parent hydrides

Normal prefix names are used to describe substituents of the B, Al, In, or Tl parent hydrides.

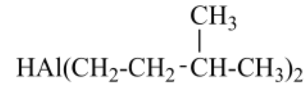
Examples:

$B(CH_3)_3$

trimethylborane (PIN)

$Al(C_2H_5)_3$

triethylalumane



$$HAl(CH_2\text{-}CH_2\text{-}\overset{\overset{CH_3}{|}}{C}H\text{-}CH_3)_2$$

bis(3-methylbutyl)alumane

$Al(O\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}CH_3)_3$

tributoxyalumane

$$CH_3\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}BH\text{-}\overset{N}{N}H\text{-}BH\text{-}\overset{N'}{N}H\text{-}BH\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}CH_3$$

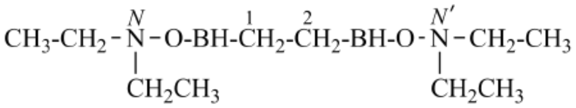
N,*N′*-bis(butylboranyl)boranediamine (PIN)

(not 1,5-dibutyltriborazane)

$$\overset{10}{C}H_3\text{-}\overset{9}{B}(CH_3)\text{-}\overset{8}{C}H_2\text{-}\overset{7}{O}\text{-}\overset{6}{C}H_2\text{-}\overset{5}{C}H_2\text{-}\overset{4}{O}\text{-}\overset{3}{C}H_2\text{-}\overset{2}{B}(CH_3)\text{-}\overset{1}{C}H_3$$

2,9-dimethyl-4,7-dioxa-2,9-diboradecane (PIN)

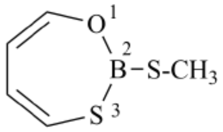
[ethane-1,2-diylbis(oxymethylene)]bis(dimethylborane)



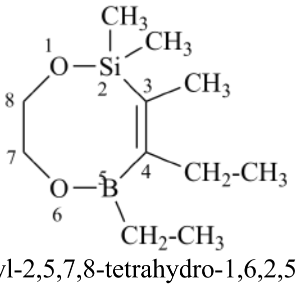
$$CH_3\text{-}CH_2\text{-}\underset{\underset{CH_2CH_3}{|}}{\overset{N}{N}}\text{-}O\text{-}BH\text{-}\overset{1}{C}H_2\text{-}\overset{2}{C}H_2\text{-}BH\text{-}O\text{-}\underset{\underset{CH_2CH_3}{|}}{\overset{N'}{N}}\text{-}CH_2\text{-}CH_3$$

N,*N′*-[ethane-1,2-diylbis(boranediyloxy)]bis(*N*-ethylethanamine) (PIN)

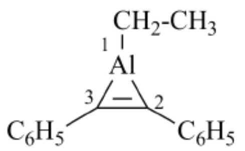
O,*O′*-[ethane-1,2-diylbis(boranediyl)]bis(*N*,*N*-diethylhydroxylamine)



2-(methylsulfanyl)-2*H*-1,3,2-oxathiaborepine (PIN)



4,5-diethyl-2,2,3-trimethyl-2,5,7,8-tetrahydro-1,6,2,5-dioxasilaborocine (PIN)



1-ethyl-2,3-diphenyl-1*H*-aluminirene

P-68.1.5.2.2 Compounds with bridging atoms or groups

Derivatives of di- and polyheteranes of the Group 13 elements, such as diborane, polyboranes, and related Al, Ga, In, and Tl congeners, are named using substitutive nomenclature. When a nonbridging hydrogen is substituted, locants, including the locant ‘1’, are used in the customary way. Bridging atoms or groups are indicated as follows:

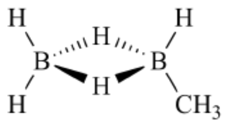
(a) a bridging substituent is indicated by adding the Greek letter μ (mu) immediately before the name of the substituent and separating its prefix name from that of the rest of the name by hyphens;

(b) two or more bridging substituents of the same kind are indicated by ‘di-μ’ or ‘bis-μ’, and so on;

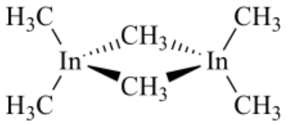
(c) bridging substituents are listed with the other substituents in alphanumerical order;

where the same substituent is present as a bridging group and as a nonbridging substituent it is cited first as a bridging substituent.

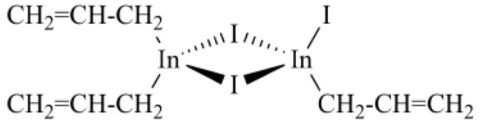
Examples:



1-methyldiborane(6) (PIN)



di-μ-methyl-tetramethyldiindigane(6)



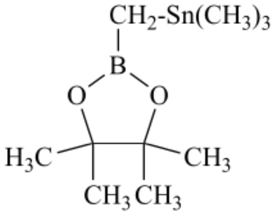
di-μ-iodo-1-iodo-1,2,2-tris(prop-2-en-1-yl)diindigane(6)

For more examples of the application of the symbol 'μ', see Rule IR-9.2.5.2 and IR-10.2.3.1, in ref. 12.

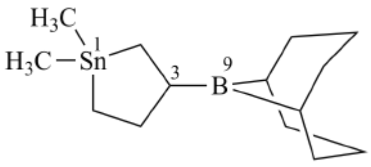
P-68.1.5.2.3 Compounds with groups of higher seniority

In the presence of groups of higher seniority, parent structures and prefixes are chosen in accordance with the seniority of classes (see P-41).

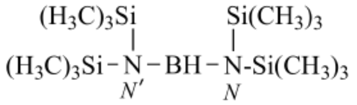
Examples:



trimethyl[(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)methyl]stannane (PIN)
(Sn is senior to B)

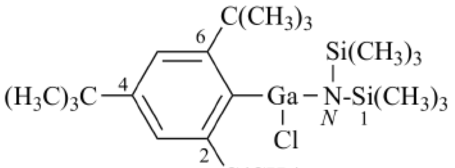


3-(9-borabicyclo[3.3.1]nonan-9-yl)-1,1-dimethylstannolane (PIN)

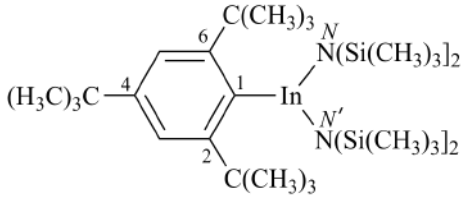


$$(\mathrm{H_3C})_3\mathrm{Si}-\underset{N'}{\overset{(\mathrm{H_3C})_3\mathrm{Si}}{\mathrm{N}}}-\mathrm{BH}-\underset{N}{\overset{\mathrm{Si(CH_3)_3}}{\mathrm{N}}}\text{-}\mathrm{Si(CH_3)_3}$$

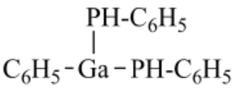
N,*N*,*N*′,*N*′-tetrakis(trimethylsilyl)boranediamine (PIN)
[not *N*,*N*′-boranediylbis[1,1,1-trimethyl-*N*-(trimethylsilyl)silanamine];
the diamine is senior to a monoamine even though 'Si' is senior to 'B' (see P-44.1.1)



N-[chloro(2,4,6-tri-*tert*-butylphenyl)gallanyl]-1,1,1-trimethyl-*N*-(trimethylsilyl)silanamine
(Si is senior to Ga)

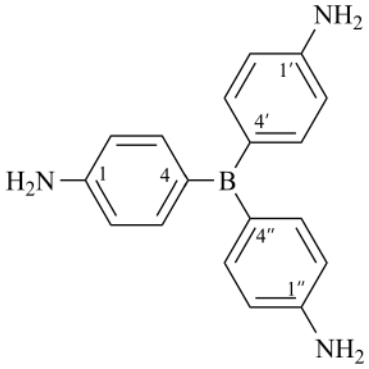


[(2,4,6-tri-*tert*-butylphenyl)-*N*,*N*,*N*′,*N*′-tetrakis(trimethylsilyl)indiganediamine
{not *N*,*N*′-[(2,4,6-tri-*tert*-butylphenyl)indiganediyl]bis[1,1,1-trimethyl-*N*-(trimethylsilyl)silanamine];
the diamine is senior to a monoamine even though Si is senior to In; see P-44.1.1}

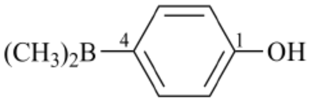


$$C_6H_5\text{-}\overset{\overset{\displaystyle PH\text{-}C_6H_5}{|}}{Ga}\text{-}PH\text{-}C_6H_5$$

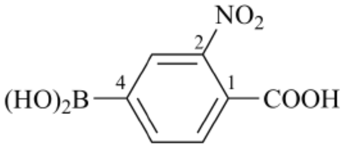
P,*P*′-(phenylgallanediyl)bis(phenylphosphane)
(P is senior to Ga)



4,4′,4″-boranetriyltrianiline (PIN; a multiplicative name)
4,4′,4″-boranetriyltris(benzen-1-amine)



4-(dimethylboranyl)phenol (PIN)



4-borono-2-nitrobenzoic acid (PIN)

$(CH_3)_3Si\text{-}BF_2$
(difluoroboranyl)tri(methyl)silane (PIN)
(Si is senior to B)
[not (trimethylsilyl)boronic difluoride; see P-67.1.2.5.2]

$Ga(S\text{-}S\text{-}CH_2\text{-}CH_3)_3$
tris(ethyldisulfanyl)gallane
tris[ethyl(dithioperoxy)]gallane

$Al(O\text{-}CO\text{-}[CH_2]_{16}\text{-}CH_3)_3$
alumanetriyl tri(octadecanoate)
(a pseudoester)

P-68.1.6 Adducts (see also P-14.8)

An adduct is a new chemical species (AB), each molecular entity of which is formed by direct combination (addition) of two separate molecular entities (A) and (B) in such a way that there may be a change of connectivity but no gain or loss of atoms in either of the molecular entities (see ref. 18). ‘Adduct’ is a general term specifically used for products of addition reactions which, whenever appropriate, should be used in preference to the less explicit term ‘complex’. Stoichiometries other than ‘1:1’ are also possible, e.g. ‘2:1’, a bis-adduct. An intramolecular adduct is formed when A and B are groups contained within the same molecular entity.

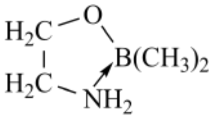
In this section Lewis adducts involving boron compounds are described based on the general principles for organic adducts given in P-14.8. The Lewis acid component is usually an organic boron compound, the electron-pair acceptor; the Lewis base component is usually, but not always, an organic nitrogen compound.

For adducts composed solely of organic compounds, the individual components are cited in the order of seniority of classes (see P-41) in formulas, no longer according to the number of species in the adduct, nor in accordance with the alphanumerical order as recommended in the 1979 Recommendations (see Rule D-1.55, ref. 1) and in the revised Nomenclature of Inorganic Chemistry, 2005 Recommendations (ref. 12).

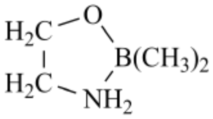
P-68.1.6.1 Structures for Lewis 'adducts'

These adducts may be separate species that are mixed at the molecular level or be attached to each other in an undefined way, in which case the components are associated with each other in the formula using a center dot. When the attachments are known, the components have been shown in three different ways, each of which has connotations to the type of nomenclature used.

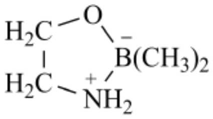
One of the fundamental principles of organic chemical nomenclature is to name the structure that is drawn, and not to ascertain what an actual electronic configuration might be. Hence, one must be prepared to name any of the following structures that might in fact be drawn.



(**I**)



(**II**)



(**III**)

Structure (**I**) shows a connection of two components using a 'dative' bond, defined in ref. 23 as follows: "The coordination bond is formed upon interaction between molecular species, one of which serves as a donor and the other as an acceptor of the electron pair to be shared in the complex formed, e.g. the N→B bond in $H_3N{\rightarrow}BH_3$. In spite of the analogy of dative bonds with covalent bonds, in that both types imply sharing a common electron pair between two vicinal atoms, the former are distinguished by their significant polarity, lesser strength, and greater length. The distinctive feature of dative bonds is that their minimum-energy rupture in the gas phase or in inert solvent follows the heterolytic bond cleavage path". Elsewhere in the discussion of the entry 'coordination' in ref. 23, this term is declared to be obsolete declaring that the origin of the bonding electrons has by itself no bearing on the character of the bond formed. Nevertheless, the use of the arrow clearly suggests that the components may be treated as separate structures and is the format most commonly used for adduct nomenclature using organic principles; hence, it is the structure used in this document for Lewis adducts.

Structure (**II**) shows a connection using a covalent bond now favored to describe a bond consisting of two electrons regardless of their origin (ref. 18). It calls for a nomenclature using coordination principles, and would be the structures used in this document for the generation of coordination names when they are given, even though such structures are not shown. To use organic principles to name a structure showing a strict covalent bond would require use of the λ-convention for the atoms involved in the connection which simply is not favored for intermediate bonding numbers.

Structure (**III**) is the formal representation of structure (**II**) showing the formal charges on the involved atoms which would be required in order to use organic principles in naming this structure.

Organic nomenclature principles would require a zwitterionic name (see P-74), which tend to be largely avoided in organic nomenclature. No zwitterionic names are given in this subsection.

In the formulas of Lewis adducts, Lewis bases, which are generally organic in nature, are cited first following the seniority order of classes of organic compounds, rings and ring systems, and of chains as indicated in Chapter P-4, followed by inorganic compounds, i.e., compounds which do not contain carbon, in order of increasing number and, if they occur in equal numbers, in alphabetical order of the first symbols of the formulas. Lewis acids are then cited in the same order. Addition compounds containing water are exceptional, in that the water is always cited last.

P-68.1.6.2 General organic method for naming Lewis adducts

Adducts (addition compounds) between neutral Lewis bases and Lewis acids are named by citing the name of each component in the order given by the formula and connecting the name of each component by an 'em' dash (see P-16.2.4.5) or by the set of connected atomic symbols separated by an 'em' dash and enclosed in parentheses. The number of molecules of each component is denoted by two methods:

(1) appropriate multiplying prefixes, except for mono; or

(2) by indicating the proportions of the species, if necessary, after the complete name by arabic numbers separated by a solidus (/) and placed in parentheses with a space in front of the first parenthesis; water, if present, is cited last in the name, and the number of water molecules per formula unit is therefore also cited last among these numerals within the parentheses.

When desired, and especially when there may be more than one possible donor or acceptor atom, the attachments are indicated in the name by italicized atomic symbols joined by an 'em' dash (see P-16.2.4.5), enclosed in parentheses, and cited between the names of each component of the adduct. Each atomic symbol refers to the component nearest to it. The names of components and the atomic symbols are cited in the sequence donor-acceptor, the locant of a component being added before the appropriate atomic symbols, as required.

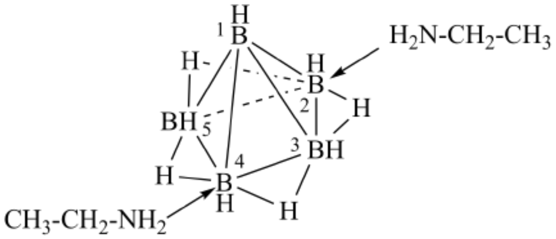
However, these 'adduct names' are not PINs; the latter are coordination or 'inorganic' names (see ref. 12). Thus, in this document, PINs for these adducts are not assigned. They will be assigned in a forthcoming document on PINs for inorganic and coordination compounds.

Examples:

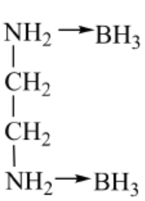
$BF_3 \cdot 2\ H_2O$
trifluoroborane—water (1/2)
(from preselected parent borane)
boron trifluoride–bis(water)
trifluoridoboron dihydrate

$(CH_3)_3N{\rightarrow}BCl_3$
N,*N*-dimethylmethanamine—trichloroborane (1/1)
trichlorido(*N*,*N*-dimethylmethanamine-κ*N*)boron

$(CH_3\text{-}CH_2)_2S{\rightarrow}H_2B\text{-}CH_3$
(ethylsulfanyl)ethane—methylborane (1/1)
[(ethylsulfanyl-κ*S*)ethane]dihydridomethanidoboron



ethanamine(*N*→*B*^{2})(*N*→*B*^{4})pentaborane(9) (2/1)
2,4-bis(ethanamine-κ*N*)-2,3:2,5:3,4:4,5-tetra-μ*H*-*nido*-pentaborane(9)

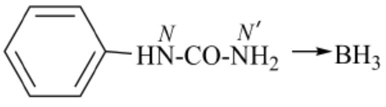


ethane-1,2-diamine—borane (1/2)
ethane-1,2-diamine—bis(borane)
μ-(ethane-1,2-diamine-1κ*N*^{1},2κ*N*^{2})-bis(trihydridoboron)

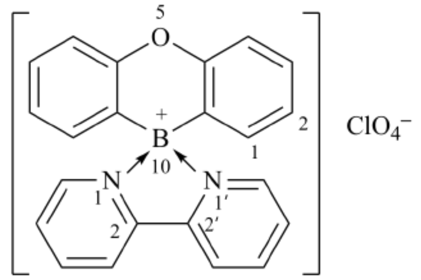
$(CH_3)_3N \cdot (CH_3)_2S \cdot B_{12}H_{10}$
N,*N*-dimethylmethanamine–(methylsulfanyl)methane–dodecaborane(10) (1/1/1)
(trimethyl)amine–(methylsulfanyl)methane–dodecaborane(10) (1/1/1)
(*N*,*N*-dimethylmethanamine)decahydrido[(methylsulfanyl)methane]dodecaboron

$H_3C\text{-}O\text{-}NH_2{\rightarrow}BH_3$
O-methylhydroxylamine(*N*—*B*)borane (1/1)
trihydrido(*O*-methylhydroxylamine-κ*N*)boron

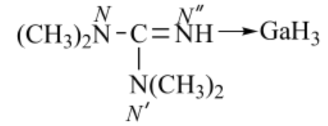
$(CH_3)_2NPF_2 \cdot B_4H_8$
N,*N*-dimethylphosphoramidous difluoride(P—B)tetraborane(8) (1/1)
(*N*,*N*-dimethylphosphoramidous difluoride-κ*P*)octahydridotetraboron



N-phenylurea(*N*′—*B*)borane (1/1)
trihydrido(*N*-phenylurea-κ*N*′)boron



2,2′-bipyridine(N^1,$N^{1'}$—*B*)-10*H*-phenoxaborin-10-ylium perchlorate
(2,2′-bipyridine-κ$^2N^1$,$N^{1'}$)[2,2′-oxybis(benzen-1-ido-κC^1)]boron(1+) perchlorate



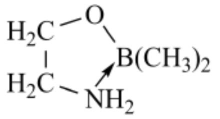
$$(CH_3)_2\overset{N}{N}-\underset{\substack{|\\ \underset{N'}{N(CH_3)_2}}}{C}=\overset{N''}{N}H \longrightarrow GaH_3$$

N,*N*,*N*′,*N*′-tetramethylguanidine(*N*″—*Ga*)gallane (1/1)
trihydrido[*N*,*N*,*N*′,*N*′-tetramethylguanidine-κ*N*″]gallium

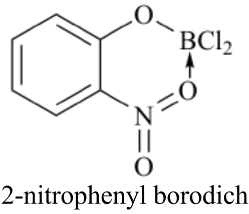
P-68.1.6.3 Intramolecular adducts

An intramolecular adduct between a group acting as a Lewis base and another group acting as a Lewis acid in the same molecule is denoted by atomic symbol pairs in the order donor-acceptor as described in Rule P-68.1.6.2, but enclosed in parentheses and cited in front of an appropriate portion of the name of the compound. A symbol denoting the proportions of the components is not required.

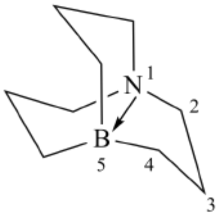
Examples:



(*N*—*B*)-2-aminoethyl dimethylborinate
(2-amino-κ*N*-ethan-1-olato-κ*O*)dimethanidoboron

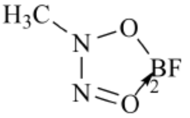


(*O*—*B*)-2-nitrophenyl borodichloridate
(*O*—*B*)dichloro(2-nitrophenoxy)borane
dichlorido(2-nitro-κ*O*-phenolato-κ*O*)boron

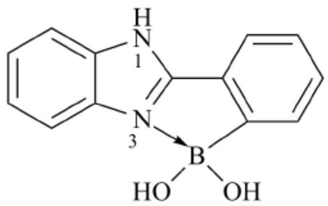


(*N*—*B*)-1-aza-5-borabicyclo[3.3.3]undecane (numbering shown)
[3,3′,3″-nitrilo-κ*N*-tris(propan-1-yl-κC^1)]boron
[3,3′,3″-nitrilo-κ*N*-tris(propan-1-ido-κC^1)]boron

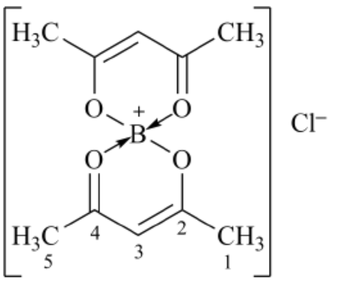
Note: If the structure is shown as a charged system, it is named as a zwitterion (see P-74.1.1).



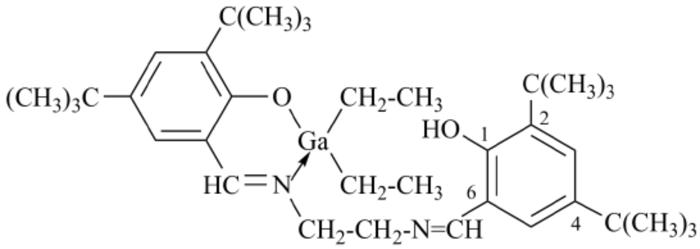
(*O*—*B*)-*N*-[(difluoroboranyl)oxy]-*N*-nitrosomethanamine
difluorido(*N*-nitroso-κ*O*-*N*-oxido-κ*O*-methanamine)boron



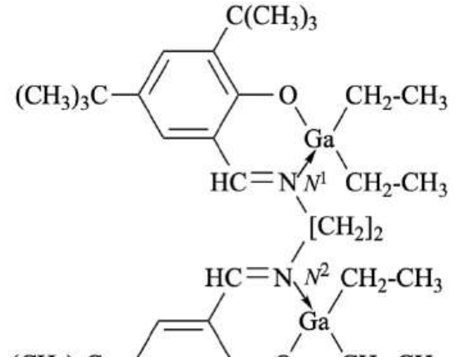
(N^3—B)[2-(1H-1,3-benzimidazol-2-yl)phenyl]boronic acid
(N^3—B)[2-(1H-benzimidazol-2-yl)phenyl]boronic acid
{not (N^3—B)-2-[(dihydroxyboranyl)phenyl]benzimidazole}
[2-(1H-1,3-benzimidazol-2-yl-κN^3)benzen-1-ido-κC^1]dihydroxidoboron
[2-(1H-benzimidazol-2-yl-κN^3)benzen-1-ido-κC^1]dihydroxidoboron



[2(*O*—*B*)]bis[(4-oxopent-2-en-2-yl)oxy]boranylium chloride
bis(4-oxo-κ*O*-pent-2-en-2-olato-κ*O*)boron(1+) chloride



2,4-di-*tert*-butyl-6-[({2-[({(*N*—*Ga*)-3,5-di-*tert*-butyl-2-[(diethylgallanyl)-oxy]phenyl}methylidene)amino]ethyl}imino)methyl]phenol
[2,4-di-*tert*-butyl-6-{[(2-{[(3,5-di-*tert*-butyl-2-hydroxyphenyl)methylidene]amino}ethyl)imino-κ*N*]methyl}phenolato-κ*O*]diethanidogallium



N^1,N^2-bis({3,5-di-*tert*-butyl-2-[(diethylgallanyl)oxy]phenyl}methylidene)-2(*N*—*Ga*)-ethane-1,2-diamine
(μ-{2,2′-[ethane-1,2-diylbis(azanylylidene-1κN^1:2κN^2-methanylylidene)bis(4,6-di-*tert*-butylphenolato-1κ*O*:2κ*O*′)]})bis[di(ethanido-1κ$^2C^1$,2κ$^2C^1$)gallium]

P-68.2 NOMENCLATURE FOR COMPOUNDS OF THE GROUP 14 ELEMENTS

P-68.2.0 Introduction

The nomenclature of carbon compounds as the basis for organic compounds, has been described in previous chapters. It is not exemplified in this Section, unless comparisons with other compounds are needed.

With the exception of silicic acid, a retained name for $Si(OH)_4$ (formerly orthosilic acid), all silicon compounds and a large number of germanium, tin, and lead compounds are named in accordance with the principles, rules and conventions of substitutive nomenclature.

Germanium, tin, and lead compounds that do not contain carbon or that cannot be named by the principles of substitutive nomenclature as defined in these recommendations for carbon compounds are named by the principles of coordination nomenclature (see ref. 12).

Suffixes are now used in accordance with the seniority of classes (see P-41) for germanium, tin, and lead compounds, which is a change from the traditional system where prefixes only were used for compounds of these elements.

P-68.2.1 Silicon, germanium, tin, and lead parent hydrides
P-68.2.2 Substituent groups derived from parent hydrides
P-68.2.3 Modification of the degree of hydrogenation
P-68.2.4 Silicic acid as a functional parent compound
P-68.2.5 Substitutive nomenclature: suffix mode
P-68.2.6 Substitutive nomenclature: prefix mode

P-68.2.1 Silicon, germanium, tin, and lead parent hydrides

P-68.2.1.1 Mononuclear and acyclic parent hydrides
P-68.2.1.2 Cyclic parent hydrides

P-68.2.1.1 Mononuclear and acyclic parent hydrides

Names of acyclic parent hydrides are formed in accordance with the general rules described in Section P-21. They are preselected names.

Examples:

$$\overset{13}{H_3Sn}\text{-}[SnH_2]_{11}\text{-}\overset{1}{SnH_3}$$

tridecastannane (preselected name)

$$\overset{5}{H_3Ge}\text{-}\overset{4}{Se}\text{-}\overset{3}{GeH_2}\text{-}\overset{2}{Se}\text{-}\overset{1}{GeH_3}$$

trigermaselenane (preselected name)

$$H_3\overset{43}{Si}\text{-}[O\text{-}SiH_2]_{20}\text{-}\overset{2}{O}\text{-}\overset{1}{SiH_3}$$

docosasiloxane (preselected name)

$$\overset{3}{H_3Pb}\text{-}\overset{2}{Te}\text{-}\overset{1}{PbH_3}$$

diplumbatellurane (preselected name)

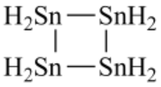
$$\overset{12}{CH_3}\text{-}\overset{11}{SiH_2}\text{-}\overset{10}{CH_2}\text{-}\overset{9}{CH_2}\text{-}\overset{8}{SiH_2}\text{-}\overset{7}{CH_2}\text{-}\overset{6}{CH_2}\text{-}\overset{5}{SiH_2}\text{-}\overset{4}{CH_2}\text{-}CH_2\text{-}\overset{2}{SiH_2}\text{-}\overset{1}{CH_3}$$

2,5,8,11-tetrasiladodecane (PIN)
ethylenebis[2-(methylsilyl)ethylsilane]

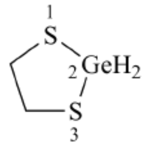
P-68.2.1.2 Cyclic parent hydrides

Names and preferred IUPAC names of cyclic parent hydrides are formed in accordance with the rules described in Sections P-22 through P-28. Those with no carbon atoms are preselected.

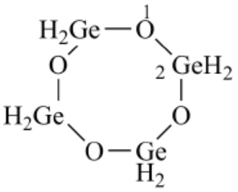
Examples:



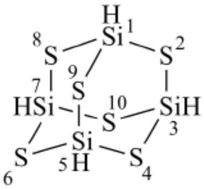
tetrastannetane (preselected name, Hantzsch-Widman name)
cyclotetrastannane



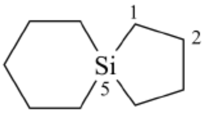
1,3,2-dithiagermolane (PIN)



1,3,5,7,2,4,6,8-tetroxatetragermocane (preselected Hantzsch-Widman name)
cyclotetragermoxane



2,4,6,8,9,10-hexathia-1,3,5,7-tetrasilaadamantane (preselected name)



5-silaspiro[4.5]decane (PIN)

P-68.2.2 Substituent groups derived from parent hydrides

Names of substituent groups $-XH_3$, $=XH_2$, and $\equiv XH$ derived from mononuclear parent hydrides where X = Si, Ge, Sn, and Pb, but not B, are formed by the method (1) described in P-29.2; all other substituent groups are named by using the general method (2) described in P-29.2.

Examples:

$-SiH_3$
silyl (preselected prefix)

$-GeH_3$
germyl (preselected prefix)

$-SnH_3$
stannyl (preselected prefix)

$-PbH_3$
plumbyl (preselected prefix)

$-SiH_2-$
silanediyl (preselected prefix)
(not silylene)

$-GeH_2-$
germanediyl (preselected prefix)
(not germylene)

$-SnH_2-$
stannanediyl (preselected prefix)
(not stannylene)

$-PbH_2-$
plumbanediyl (preselected prefix)
(not plumbylene)

$=SiH_2$
silylidene (preselected prefix)
(not silylene)

$=PbH_2$
plumbylidene (preselected prefix)
(not plumbylene)

$\equiv GeH$
germylidyne (preselected prefix)

$\equiv SnH$
stannylidyne (preselected prefix)
(not stannylene)

$\equiv SiH$
silylidyne (preselected prefix)

$-SiH=$
silanylylidene (preselected prefix)

$-SnH<$
stannanetriyl (preselected prefix)

$=Ge=$
germanediylidene (preselected prefix)

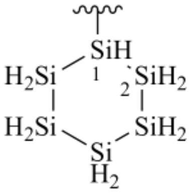
$>Pb<$
plumbanetetrayl (preselected prefix)

$H_3Si\text{-}SiH_2-$
disilanyl (preselected prefix)
(not disilyl)

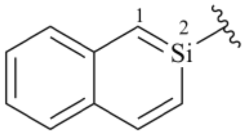
$\overset{3}{H_3Ge}\text{-}\overset{2}{GeH_2}\text{-}\overset{1}{GeH}=$
trigerman-1-ylidene (preselected prefix)

$-H_2\overset{1}{Si}\text{-}\overset{2}{Si}H_2-$
disilane-1,2-diyl (preselected prefix)

$\overset{2}{Si}H_3\text{-}\overset{1}{Si}H<$
disilane-1,1-diyl (preselected prefix)



hexasilinanyl (preselected prefix)
cyclohexasilanyl



2-benzosilin-2-yl (preferred prefix)

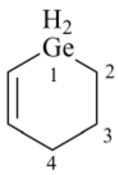
P-68.2.3 Modification of the degree of hydrogenation

Double bonds are denoted by the ‘ene’ ending, as described in Section P-31.1, and saturation of double bonds of mancude structures by ‘hydro’ prefixes as indicated in P-31.2.

In these recommendations, the prefixes ‘hydro’ and ‘dehydro’ are detachable, but are not included in the category of alphabetized detachable prefixes (see P-14.4; see also P-15.1.5.2, P-31.2, P-58.2). This is a change from recommendations in earlier editions (ref. 1, 2).

Examples:

$H_2Ge=GeH_2$
digermene (preselected name)



1,2,3,4-tetrahydrogermine (PIN)

P-68.2.4 Silicic acid as functional parent compound

The nomenclature of silicic acid (formerly orthosilicic acid) has been discussed in Section P-67.1.2. Silicic acid is modified only by prefixes to denote functional replacement by chalcogen atoms. Functional replacement by other atoms or groups is not recommended. Names of salts, esters, and anhydrides are derived from the retained name silicic acid. Amides of silicic acid are classified as amines. Hydrazides of silicic acid are considered as derivatives of hydrazine.

Names of substituent groups derived from silicic acid are formed on the basis of the parent hydride ‘silane’ (see P-67.1.4.2).

Examples:

$(HO)_3Si–$
trihydroxysilyl (preselected name)

$(HS)(HO)_2Si–$
dihydroxy(sulfanyl)silyl (preselected name)

$Si(NH_2)_4$
silanetetramine (preselected name)
(not silicic tetraamide)

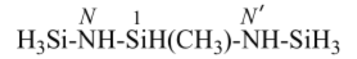
$Si(NH\text{-}NH_2)_4$
1,1′,1″,1‴-silanetetrayltetrahydrazine (preselected name)
(not silicic tetrahydrazide)

P-68.2.5 Substitutive nomenclature: suffix mode

Traditionally, silicon compounds were denoted by suffixes or prefixes; germanium, tin, and lead compounds were denoted only by prefixes. Full systematization is recommended to use suffixes, when available, to generate preferred names, in accordance with the seniority order of suffixes, and the seniority of suffixes over prefixes.

Examples:

$CH_3\text{-}Si(NH_2)_3$
methylsilanetriamine (PIN)



$\mathrm{H_3Si}\text{-}\overset{N}{\mathrm{NH}}\text{-}\overset{1}{\mathrm{Si}}\mathrm{H(CH_3)}\text{-}\overset{N'}{\mathrm{NH}}\text{-}\mathrm{SiH_3}$

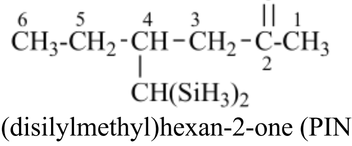
1-methyl-*N*,*N′*-disilylsilanediamine (PIN)
(not 3-methyltrisilazane)

$(CH_3)_2Si(OH)_2$
dimethylsilanediol (PIN)

$CH_3\text{-}NH\text{-}Si(OH)_3$
(methylamino)silanetriol (PIN)

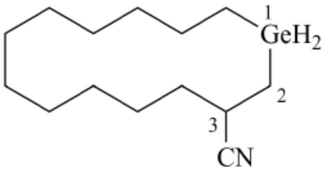
$(CH_3)_3Si\text{-}COOH$
trimethylsilanecarboxylic acid (PIN)

$CH_3\text{-}GeH_2\text{-}SH$
methylgermanethiol (PIN)
methyl(sulfanyl)germane

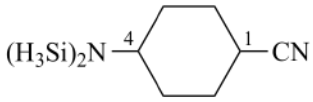


$\overset{6}{\mathrm{CH_3}}\text{-}\overset{5}{\mathrm{CH_2}}\text{-}\underset{\mathrm{CH(SiH_3)_2}}{\overset{4}{\mathrm{CH}}}\text{-}\overset{3}{\mathrm{CH_2}}\text{-}\underset{2}{\overset{\mathrm{O}}{\overset{\|}{\mathrm{C}}}}\text{-}\overset{1}{\mathrm{CH_3}}$

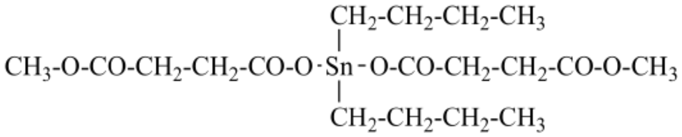
4-(disilylmethyl)hexan-2-one (PIN)
4-[bis(silanyl)methyl]hexan-2-one



1-germacyclotetradecane-3-carbonitrile (PIN)
3-cyano-1-germacyclotetradecane



4-(disilylamino)cyclohexane-1-carbonitrile (PIN)
4-[bis(silanyl)amino]cyclohexane-1-carbonitrile



$$CH_3\text{-}O\text{-}CO\text{-}CH_2\text{-}CH_2\text{-}CO\text{-}O\text{-}\overset{CH_2\text{-}CH_2\text{-}CH_2\text{-}CH_3}{\underset{CH_2\text{-}CH_2\text{-}CH_2\text{-}CH_3}{Sn}}\text{-}O\text{-}CO\text{-}CH_2\text{-}CH_2\text{-}CO\text{-}O\text{-}CH_3$$

dimethyl dibutylstannanediyl dibutanedioate (PIN; see P-65.6.3.3.4)
dibutylbis[(4-methoxy-4-oxobutanoyl)oxy]stannane

$[(CH_3)_3Si]_2CH\text{-}SnH(OH)\text{-}CH[Si(CH_3)_3]_2$
bis[bis(trimethylsilyl)methyl]stannanol (PIN)
[(hydroxystannanediyl)dimethanetriyl]tetrakis(trimethylsilane)

P-68.2.6 Substitutive nomenclature: prefix mode

Prefixes are used as recommended for substitutive nomenclature in two ways.

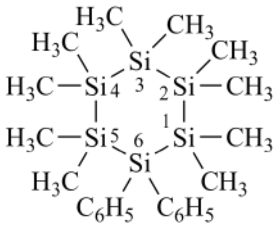
P-68.2.6.1 Subsitituted parent hydrides
P-68.2.6.2 Seniority of the Group 14 elements

When required, parent structures and prefixes are chosen in accordance with the seniority of classes (see P-41).

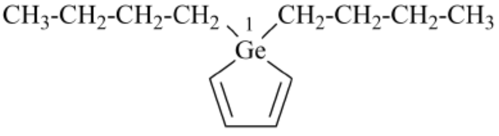
P-68.2.6.1 Substituted parent hydrides

Examples:

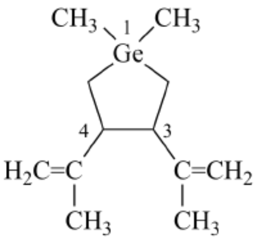
$CH_3\text{-}[CH_2]_{11}\text{-}SiH_2\text{-}[CH_2]_{11}\text{-}CH_3$
di(dodecyl)silane (PIN)



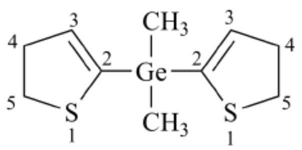
1,1,2,2,3,3,4,4,5,5-decamethyl-6,6-diphenylhexasilinane (PIN; Hantzsch-Widman name)
1,1,2,2,3,3,4,4,5,5-decamethyl-6,6-diphenylcyclohexasilane



1,1-dibutyl-1*H*-germole (PIN)
(note the indicated hydrogen atom)



1,1-dimethyl-3,4-di(prop-1-en-2-yl)germolane (PIN)
3,4-diisopropenyl-1,1-dimethylgermolane

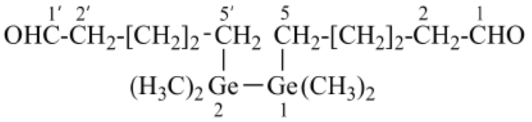


bis(4,5-dihydrothiophen-2-yl)di(methyl)germane (PIN)
(Ge is senior to S)

P-68.2.6.2 Seniority of the Group 14 elements

In the presence of groups of higher seniority, parent structures and prefixes are chosen according to the order of seniority (see P-41 and P-44) and the rules for selection of a preferred name (see P-45).

Examples:

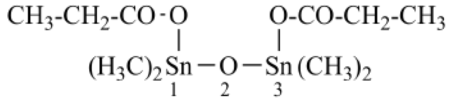


$$\begin{array}{c} \overset{1'}{\text{OHC}}\text{-}\overset{2'}{\text{CH}_2}\text{-[CH}_2]_2\text{-}\overset{5'}{\text{CH}_2}\ \ \overset{5}{\text{CH}_2}\text{-[CH}_2]_2\text{-}\overset{2}{\text{CH}_2}\text{-}\overset{1}{\text{CHO}} \\ (\text{H}_3\text{C})_2\underset{2}{\text{Ge}}-\underset{1}{\text{Ge}}(\text{CH}_3)_2 \end{array}$$

5,5′-(1,1,2,2-tetramethyldigermane-1,2-diyl)di(pentanal) (PIN)

$(\text{CH}_3\text{-CH}_2\text{-O})_3\text{Ge-}\overset{3}{\text{C}}\text{H}_2\text{-}\overset{2}{\text{C}}\text{H}_2\text{-}\overset{1}{\text{C}}\text{OO-CH}_3$

methyl 3-(triethoxygermyl)propanoate (PIN)



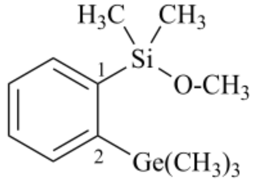
$$\begin{array}{c} \text{CH}_3\text{-CH}_2\text{-CO-O}\qquad\text{O-CO-CH}_2\text{-CH}_3 \\ (\text{H}_3\text{C})_2\underset{1}{\text{Sn}}-\underset{2}{\text{O}}-\underset{3}{\text{Sn}}(\text{CH}_3)_2 \end{array}$$

1,1,3,3-tetramethyldistannoxane-1,3-diyl dipropanoate (PIN)

$\text{H}_3\text{Pb-CH}_2\text{-PbH}_2\text{-CH}_2\text{-PbH}_3$

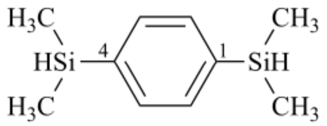
[plumbanediylbis(methylene)]bis(plumbane) (PIN)

bis(plumbylmethyl)plumbane

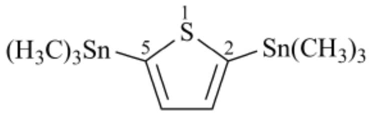


methoxydi(methyl)[2-(trimethylgermyl)phenyl]silane (PIN)

(Si is senior to Ge)



(1,4-phenylene)bis(dimethylsilane) (PIN)



(thiophene-2,5-diyl)bis(trimethylstannane) (PIN)

(Sn preferred to S, see P-41)

$[(\text{CH}_3)_3\text{Si}]_2\text{CH-SnH(OH)-CH}[\text{Si}(\text{CH}_3)_3]_2$

bis[bis(trimethylsilyl)methyl]stannanol (PIN)

[(hydroxystannanediyl)dimethanetriyl]tetrakis(trimethylsilane)

[Decided by P-41 table 4.1 class 17, not class 26 or class 28]

P-68.3 NOMENCLATURE FOR COMPOUNDS OF THE GROUP 15 ELEMENTS

For the purposes of nomenclature, compounds of the Group 15 elements are divided into three categories:

(1) Nitrogen compounds are named as amines and imines (see P-62), amides, hydrazides, imides, amidines, amidrazones, hydrazidines, nitriles and cyanides (see P-66), or substitutively on the basis of parent hydrides, such as hydrazine, triazane, etc., or as derivatives of functional parent compounds, such as hydroxylamine (see P-68.3.1.1). Because of similarities, azonic HN(O)(OH)_2 and azinic acids $\text{H}_2\text{N(O)(OH)}$, are discussed in Section P-67 along with the P, As, and Sb oxoacids.

(2) Phosphorus, arsenic, and antimony compounds are discussed together in P-68.3.2 because of the importance of functional class nomenclature based on their acids used as functional parents. Other compounds are named substitutively on the basis of parent hydrides.

(3) Bismuth compounds that contain carbon and that can be named by the principles of substitutive nomenclature as described in these recommendations are named by substitution of parent hydrides, such as bismuthane, BiH_3 (see P-68.3.3). Bismuth compounds that do not contain carbon or that cannot be named by the principles of substitutive nomenclature as defined in these recommendations for carbon compounds are named by the principles of coordination nomenclature (see ref. 12).

P-68.3.1 Nitrogen compounds

P-68.3.1.0 Introduction
P-68.3.1.1 Hydroxylamines, oximes, and nitrolic acids and nitrosolic acids
P-68.3.1.2 Hydrazine and related compounds: hydrazones, azines, semicarbazides, semicarbazones, and carbonohydrazides
P-68.3.1.3 Diazene and related compounds
P-68.3.1.4 Polyazanes

P-68.3.1.0 Introduction

Many acyclic nitrogen compounds have retained names or functional class names. These names are retained for use in general nomenclature, but for most acyclic nitrogen compounds preferred IUPAC names are formed systematically. Hydroxylamine is a preselected name and urea, guanidine, and formazan are retained as preferred IUPAC names. Other retained names have been inserted into systematic substitutive nomenclature; oxime is retained only as a functional class name.

P-68.3.1.1 Hydroxylamines, oximes, and nitrolic and nitrosolic acids

Compounds containing a nitrogen atom which belong to classes identified as hydroxylamines, oximes, and nitrolic and nitrosolic acids are illustrated here. Nitro and nitroso compounds, isocyanates, and isonitriles were discussed in Section P-61.

The class name 'hydroxylamine', a preselected name, is also used as a functional parent compound. The class name 'oxime' is used as a functional class modifier. Nitrolic and nitrosolic acids are named as oximes of pseudoketones.

P-68.3.1.1.1 Hydroxylamines
P-68.3.1.1.2 Oximes
P-68.3.1.1.3 Nitrolic and nitrosolic acids

P-68.3.1.1.1 Hydroxylamines

The retained name 'hydroxylamine' is a preselected name and designates the structure H_2N-OH. It is a functional parent compound allowing full substitution even, as an exception, on the oxygen atom. Substitution on the nitrogen or the oxygen atom of hydroxylamine may create a function senior to hydroxylamine, justifying a systematic name based on a higher class denoting the new function.

P-68.3.1.1.1.1 Substituted hydroxylamines of the type R-NH-OH or RR′N-OH are named as *N*-derivatives of the senior amine.

Examples:

CH_3-NH-OH
N-hydroxymethanamine (PIN)
N-methylhydroxylamine

$(CH_3)_2N$-OH
N-hydroxy-*N*-methylmethanamine (PIN)
N,*N*-dimethylhydroxylamine

H_3Si-NH-OH
N-hydroxysilanamine (preselected name)
N-silylhydroxylamine

H_2B-NH-OH
N-hydroxyboranamine (preselected name)
N-boranylhydroxylamine

N-Substitution of hydroxylamine by acyl groups generates hydroxamic acids that are now named as *N*-hydroxyamides (see P-65.1.3.4).

Examples:

CH_3-CO-NH-OH
N-hydroxyacetamide (PIN)
(not acetohydroxamic acid)

CH_3-SO_2-NH-OH
N-hydroxymethanesulfonamide (PIN)

CH_3-CH_2-CO-NH-OH
N-hydroxypropanamide (PIN)

propanohydroxamic acid
propionohydroxamic acid

P-68.3.1.1.1.2 Substitution on the oxygen atom of hydroxylamine

Substitution of hydroxylamine on the oxygen atom by hydrocarbyl or acyl groups is expressed as *O*-substitution. Names such as ‘alkyloxyamines’ are not recommended and the class ‘peroxyamide’ has never been recognized.

Examples:

$H_2N\text{-}O\text{-}CH_3$
O-methylhydroxylamine (PIN)
(not methoxyamine)

$H_2N\text{-}O\text{-}C_6H_5$
O-phenylhydroxylamine (PIN)
(not phenoxyamine)

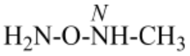
$H_2N\text{-}O\text{-}CH_2\text{-}CH_2\text{-}O\text{-}NH_2$
O,*O*′-(ethane-1,2-diyl)bis(hydroxylamine) (PIN)

$H_2N\text{-}O\text{-}CO\text{-}C_6H_5$
aminooxy(phenyl)methanone (PIN)
O-benzoylhydroxylamine
(not azanyl benzoate)

$H_2N\text{-}O\text{-}SO\text{-}CH_3$
O-(methanesulfinyl)hydroxylamine (PIN)
(not azanyl methanesulfinate)

O-Substitution of hydroxylamine by –NHR or –NRR′ leads to *N*-(aminooxy)amines not derivatives of diazoxane.

Example:



$H_2N\text{-}O\text{-}\overset{N}{N}H\text{-}CH_3$

N-(aminooxy)methanamine (PIN)
(not 1-methyldiazoxane)

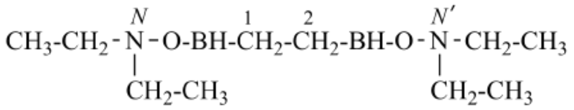
P-68.3.1.1.1.3 *N*,*O*-Disubstitution of hydroxylamine

Substitution of hydroxylamine on both nitrogen and oxygen atoms leads to *O*-substituted amines.

Examples:

$CH_3\text{-}NH\text{-}O\text{-}CH_3$
N-methoxymethanamine (PIN)
N,*O*-dimethylhydroxylamine

$C_6H_5\text{-}NH\text{-}O\text{-}CH_2\text{-}CH_3$
N-ethoxyaniline (PIN)
O-ethyl-*N*-phenylhydroxylamine



$CH_3\text{-}CH_2\text{-}\underset{\displaystyle | \atop CH_2\text{-}CH_3}{\overset{N}{N}}\text{-}O\text{-}BH\text{-}\overset{1}{C}H_2\text{-}\overset{2}{C}H_2\text{-}BH\text{-}O\text{-}\underset{\displaystyle | \atop CH_2\text{-}CH_3}{\overset{N'}{N}}\text{-}CH_2\text{-}CH_3$

N,*N*′-[ethane-1,2-diylbis(boranediyloxy)]bis(*N*-ethylethanamine) (PIN)
O,*O*′-[ethane-1,2-diylbis(boranediyl)]bis(*N*,*N*-diethylhydroxylamine)

Note: Skeletal (‘a’) replacement nomenclature cannot be used for this compound because the amine characteristic group would not be recognized and an ‘a’ chain cannot terminate on an oxygen atom.

P-68.3.1.1.1.4 Substitution of hydroxylamine by characteristic groups normally expressed as suffixes

Hydroxylamine is a functional parent to which, exceptionally, suffixes expressing characteristic groups, such as acids, amides, etc., can be attached to the oxygen atom. In names, the locant ‘*O*’ is placed in front of the suffix.

Attachment of characteristic groups to the nitrogen atom generally leads to compounds of higher function.

Examples:

$H_2N-O-SO_2-OH$
hydroxylamine-*O*-sulfonic acid (preselected name)
(not azanyl hydrogen sulfate)

$H_2N-O-COOH$
hydroxylamine-*O*-carboxylic acid (PIN)
(not azanyl hydrogen carbonate)

$H_2N-O-CO-NH_2$
hydroxylamine-*O*-carboxamide (PIN)
(not azanyl carbamate)

P-68.3.1.1.1.5 Hydroxylamine expressed as prefixes

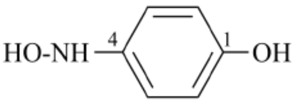
In the presence of a characteristic group having priority for citation as suffix or in the presence of a senior parent hydride, appropriate compound or complex prefixes are used:

–NH-OH
hydroxyamino (preselected prefix)

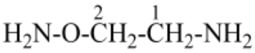
>N-OH
hydroxyazanediyl (preselected prefix)

$–O-NH_2$
aminooxy (preselected prefix)
(note that there is no elision of the final letter ‘o’ of amino)

Examples:



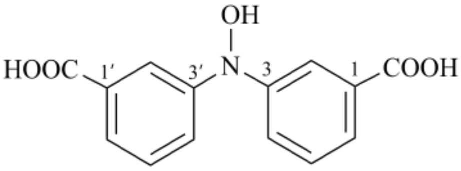
4-(hydroxyamino)phenol (PIN)



$H_2N-O-\overset{2}{C}H_2-\overset{1}{C}H_2-NH_2$

2-(aminooxy)ethan-1-amine (PIN)

$H_2N-NH-CH_2-O-NH_2$
[(aminooxy)methyl]hydrazine (PIN)



3,3′-(hydroxyazanediyl)dibenzoic acid (PIN)

P-68.3.1.1.1.6 Chalcogen analogues of hydroxylamine

Chalcogen analogues of hydroxylamine are denoted by the appropriate functional replacement prefix ‘thio’, ‘seleno’, or ‘telluro’. Parentheses are sometimes required to avoid the possibility of ambiguity. Substitution follows the principles given above for naming derivatives of hydroxylamine.

Examples:

H_2N-SH
thiohydroxylamine (preselected name)

$CH_3-NH-SH$
N-sulfanylmethanamine (PIN)
N-methyl(thiohydroxylamine)

$CH_3-CO-NH-SH$
N-sulfanylacetamide (PIN)

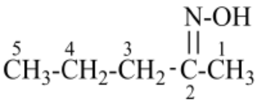
$H_2N-S-CH_3$
S-methyl(thiohydroxylamine) (PIN)

P-68.3.1.1.2 Oximes

Compounds having the general structure R-CH=N-OH or RR′C=N-OH have the class name ‘oxime’ and have been further classified as ‘aldoximes’ and ‘ketoximes’, respectively. For general nomenclature they are named according to the principles of functional class nomenclature by placing the class name ‘oxime’ as a separate word after the name of the aldehyde or ketone. Preferred IUPAC names are formed substitutively as *N*-hydroxy derivatives of imines. Compounds containing the group =N-OR are named substitutively as alkoxy substituted imines. In the presence of a characteristic group having priority for citation as a suffix, in substitutive nomenclature oximes are designated by the prefix ‘hydroxyimino’.

In these recommendations preferred IUPAC names for oximes are generated substitutively as *N*-hydroxy derivatives of imines rather than by functional class nomenclature as in previous recommendations.

Examples:

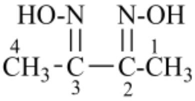


$\overset{5}{C}H_3-\overset{4}{C}H_2-\overset{3}{C}H_2-\underset{2}{\overset{\overset{N-OH}{||}}{C}}-\overset{1}{C}H_3$

N-hydroxypentan-2-imine (PIN)
(pentan-2-ylidene)hydroxylamine
pentan-2-one oxime

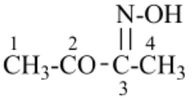
$\overset{3}{C}H_3-\overset{2}{C}H_2-\overset{1}{C}H=\overset{N}{N}-O-CH_2-CH_3$

N-ethoxypropan-1-imine (PIN)
propanal *O*-ethyloxime



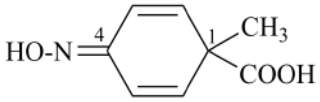
$\overset{4}{C}H_3-\underset{3}{\overset{\overset{HO-N}{||}}{C}}-\underset{2}{\overset{\overset{N-OH}{||}}{C}}-\overset{1}{C}H_3$

N^2,N^3-dihydroxybutane-2,3-diimine (PIN)
(butane-2,3-diylidene)bis(hydroxylamine)
butane-2,3-dione dioxime

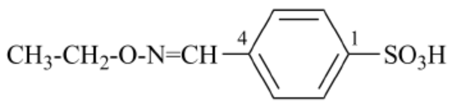


$\overset{1}{C}H_3-\overset{2}{C}O-\underset{3}{\overset{\overset{N-OH}{||}}{C}}-\overset{4}{C}H_3$

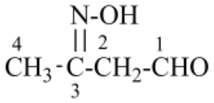
3-(hydroxyimino)butan-2-one (PIN)
butane-2,3-dione oxime



4-(hydroxyimino)-1-methylcyclohexa-2,5-diene-1-carboxylic acid (PIN)

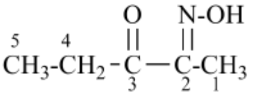


4-[(ethoxyimino)methyl]benzene-1-sulfonic acid (PIN)



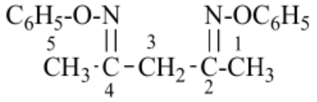
$\overset{4}{C}H_3-\underset{3}{\overset{\overset{N-OH}{||}}{C}}-\overset{2}{C}H_2-\overset{1}{C}HO$

3-(hydroxyimino)butanal (PIN)



$\overset{5}{C}H_3-\overset{4}{C}H_2-\underset{3}{\overset{\overset{O}{||}}{C}}-\underset{2}{\overset{\overset{N-OH}{||}}{C}}-\underset{1}{C}H_3$

2-(hydroxyimino)pentan-3-one (PIN)
pentane-2,3-dione 2-oxime



$\overset{5}{C}H_3-\underset{4}{\overset{\overset{C_6H_5-O-N}{||}}{C}}-\overset{3}{C}H_2-\underset{2}{\overset{\overset{N-OC_6H_5}{||}}{C}}-\overset{1}{C}H_3$

N^2,N^4-diphenoxypentane-2,4-diimine (PIN)
pentane-2,4-dione bis(*O*-phenyloxime)

P-68.3.1.1.3 Nitrolic and nitrosolic acids

Compounds having the general structures R-C(=NOH)-NO_2 and R-C(=NOH)-NO are called generically ‘nitrolic acids’ and ‘nitrosolic acids’, respectively. They are named substitutively for general nomenclature as oximes of pseudoketones. Preferred IUPAC names are formed as described above for ‘oximes’ (see P-68.3.1.1.2). Traditionally, they were named by functional class nomenclature as oximes of aldehydes substituted in position 1 by a nitro or nitroso group.

Examples:

$\overset{3}{C}H_3-\overset{2}{C}H_2-\overset{1}{C}(=\overset{N}{N}OH)-NO_2$
N-hydroxy-1-nitropropan-1-imine (PIN)
N-(1-nitropropylidene)hydroxylamine
1-nitropropanal oxime
1-nitropropan-1-one oxime

$\overset{2}{C}H_3-\overset{1}{C}(=\overset{N}{N}OH)-NO$
N-hydroxy-1-nitrosoethan-1-imine (PIN)
N-(1-nitrosoethylidene)hydroxylamine (PIN)
1-nitrosoacetaldehyde oxime)
1-nitrosoethan-1-one oxime

P-68.3.1.2 Hydrazine and related compounds: hydrazones, azines, semicarbazides, semicarbazones, and carbonohydrazides

P-68.3.1.2.1 Hydrazine and derivatives

Hydrazine is a retained name describing the structure H_2N-NH_2; it is a preselected name and is preferred to the systematic heterane name ‘diazane’.

Substituent groups derived from hydrazine are named systematically:

Preselected prefixes derived from the preselected parent hydride hydrazine are now formed systematically from hydrazine. For H_2N-NH- ‘hydrazinyl’; for $H_2N-N=$ ‘hydrazinylidene’; for =N-N= ‘hydrazinediylidene’; and for –NH-NH– ‘hydrazine-1,2-diyl’. The traditional names ‘hydrazino’, ‘hydrazono’, ‘azino’, and ‘hydrazo’, respectively, are no longer recommended, even for general nomenclature.

H_2N-NH-
hydrazinyl (preselected prefix)
diazanyl
(not hydrazino)

$H_2N-N=$
hydrazinylidene (preselected prefix)
diazanylidene
(not hydrazono)

=N-N=
hydrazinediylidene (preselected prefix)
diazanediylidene
(not azino)

–NH-NH–
hydrazine-1,2-diyl (preselected prefix)
diazane-1,2-diyl
(not hydrazo)

As a parent hydride, hydrazine is numbered by numerical locants, 1 and 2, not *N* and *N*′. Hydrazine is substituted by hydrocarbyl groups and characteristic groups expressed by suffixes and prefixes.

Examples:

$(CH_3)_2\overset{1}{N}-\overset{2}{N}H_2$
1,1-dimethylhydrazine (PIN)

$C_6H_5-NH-NH_2$
phenylhydrazine (PIN)

$H_2N-NH-\overset{1}{C}H_2-\overset{N}{N}H_2$
1-hydrazinylmethanamine (PIN)
(see also P-62.2.1.2)

$H_2N\text{-}NH\text{-}COOH$
hydrazinecarboxylic acid (PIN)
(not carbazic acid)

$F_2N\text{-}NF_2$
tetrafluorohydrazine
(from preselected name hydrazine)

$H_2N\text{-}NH\text{-}CH_2\text{-}CN$
hydrazinylacetonitrile (PIN)

$H_2N\text{-}CO\text{-}CH_2\text{-}\overset{3}{C}H_2\text{-}NH\text{-}NH\text{-}\overset{3'}{C}H_2\text{-}CH_2\text{-}CO\text{-}$
3,3′-(hydrazine-1,2-diyl)dipropanamide (PIN)
(not 3,3′-hydrazodipropanamide)

P-68.3.1.2.2 Hydrazones

Compounds having the general structure $RCH{=}N\text{-}NH_2$ or $RR'C{=}N\text{-}NH_2$ are called ‘hydrazones’ and are named in two ways:

(1) substitutively as derivatives of the parent hydride ‘hydrazine’, $H_2N\text{-}NH_2$;

(2) by functional class nomenclature using the class name ‘hydrazone’.

Method (1) generates preferred IUPAC names.

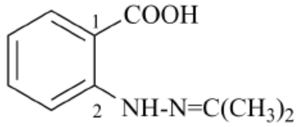
In these recommendations preferred IUPAC names for hydrazones are generated substitutively as ‘ylidene’ derivatives of hydrazine rather than by functional class nomenclature as in previous recommendations.

Examples:

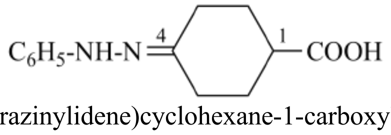
$CH_3\text{-}CH_2\text{-}CH{=}\overset{1}{N}\text{-}\overset{2}{N}H_2$
propylidenehydrazine (PIN)
propanal hydrazone

$(CH_3)_2N\text{-}N{=}C(CH_3)_2$
1,1-dimethyl-2-(propan-2-ylidene)hydrazine (PIN)
1,1-dimethyl-2-(1-methylethylidene)hydrazine
acetone dimethylhydrazone

$C_6H_5\text{-}NH\text{-}N{=}CH\text{-}CH{=}N\text{-}NH\text{-}C_6H_5$
1,1′-ethanediylidenebis(2-phenylhydrazine) (PIN)
ethane-1,2-dione bis(phenylhydrazone)



2-[(propan-2-ylidene)hydrazinyl]benzoic acid (PIN)
2-[(1-methylethylidene)hydrazinyl]benzoic acid



4-(phenylhydrazinylidene)cyclohexane-1-carboxylic acid (PIN)

P-68.3.1.2.3 Azines

P-68.3.1.2.3.1 Compounds having the general structure $R\text{-}CH{=}N\text{-}N{=}CH\text{-}R$ or $RR'C{=}N\text{-}N{=}RR'$ are called ‘azines’ and are named in two ways:

(1) substitutively, as derivatives of hydrazine;

(2) by functional class nomenclature using the class name ‘azine’.

Method (1) leads to preferred IUPAC names.

In these recommendations preferred IUPAC names for azines are generated substitutively as ‘ylidene’ derivatives of hydrazine rather than by functional class nomenclature as in previous recommendations.

Example:

$$(CH_3)_2C=\overset{1}{N}\text{-}\overset{2}{N}=C(CH_3)_2$$

di(propan-2-ylidene)hydrazine (PIN)
bis(1-methylethylidene)hydrazine
acetone azine

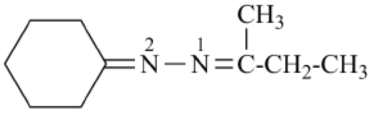
P-68.3.1.2.3.2 Azines are symmetrical derivatives of hydrazine. When this condition is not fulfilled, compounds having the structures R-CH=N-N=CH-R′ or RRC=N-N=CR′R′, are named in two ways:

(1) as unsymmetrical derivatives of hydrazine;

(2) as ‘ylidenehydrazones’ of the preferred ketone or aldehyde.

Method (1) generates preferred IUPAC names.

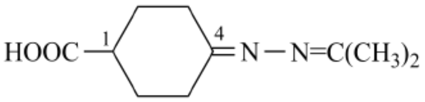
Example:



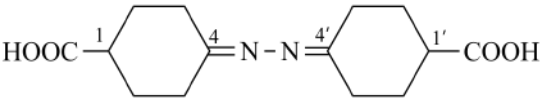
(butan-2-ylidene)(cyclohexylidene)hydrazine (PIN)
cyclohexylidene(1-methylpropylidene)hydrazine
cyclohexanone butan-2-ylidenehydrazone

P-68.3.1.2.3.3 In the presence of functions having seniority the prefix ‘hydrazinylidene’ is used substitutively, and in multiplicative nomenclature the prefix ‘hydrazinediylidene’ is used.

Examples:



4-[(propan-2-ylidene)hydrazinylidene]cyclohexane-1-carboxylic acid (PIN)
4-[(1-methylethylidene)hydrazinylidene]cyclohexane-1-carboxylic acid



4,4′-hydrazinediylidenedi(cyclohexane-1-carboxylic acid) (PIN)

P-68.3.1.2.4 Semicarbazides

Semicarbazide is the amide of ‘hydrazinecarboxylic acid’. As acids and amides expressed by suffixes are senior to acids or amides modified by functional replacement, these names are senior to ‘carbonohydrazidic acid’ and ‘carbonohydrazidic amide’.

Semicarbazide is the traditional name for the compound H_2N-NH-CO-NH_2, systematically named ‘hydrazinecarboxamide’. The systematic name is the preferred IUPAC name. The usual numbering for amides is recommended for the systematic name; special numbering is characteristic for the name semicarbazide.

$$H_2\overset{2}{N}\text{-}\overset{1}{N}H\text{-}CO\text{-}\overset{N}{N}H_2$$

hydrazinecarboxamide (PIN)

$$H_2\overset{1}{N}\text{-}\overset{2}{N}H\text{-}\overset{3}{C}O\text{-}\overset{4}{N}H_2$$

semicarbazide

Numerical locants are no longer used for the parent name semicarbazide in preferred IUPAC names.

Examples:

$$H_2\overset{2}{N}\text{-}\overset{1}{N}H\text{-}CO\text{-}\overset{N}{N}H\text{-}C_6H_5$$

N-phenylhydrazinecarboxamide (PIN)
4-phenylsemicarbazide

$$H_2\overset{2}{N}\text{-}\overset{1}{N}(CH_3)\text{-}CO\text{-}\overset{N}{N}H\text{-}CH_3$$

N,1-dimethylhydrazine-1-carboxamide (PIN)
2,4-dimethylsemicarbazide

As a prefix, the –HN-NH-CO-NH2 group is called ‘semicarbazido’, ‘2-carbamoylhydrazin-1-yl’ (preferred prefix), or ‘2-(aminocarbonyl)hydrazin-1-yl’.

Example:

$$H_2N\text{-}CO\text{-}NH\text{-}NH\text{-}\overset{3}{C}H_2\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}OOH$$

3-(2-carbamoylhydrazin-1-yl)propanoic acid (PIN)

Chalcogen analogues are named systematically as described for amides or by functional replacement nomenclature using the class term ‘semicarbazide’ modified by the replacement prefixes ‘thio’, ‘seleno’, and ‘telluro’; for example, ‘thiosemicarbazide’.

$$H_2\overset{2}{N}\text{-}\overset{1}{N}H\text{-}CSe\text{-}\overset{\mathit{N}}{N}H_2$$

hydrazinecarboselenoamide (PIN)

$$H_2\overset{1}{N}\text{-}\overset{2}{N}H\text{-}\overset{3}{C}Se\text{-}\overset{4}{N}H_2$$

selenosemicarbazide

P-68.3.1.2.5 Semicarbazones

Compounds with the structure R-CH=N-NH-CO-NR′R″ or RR′C=N-NH-CO-NR″R‴ are generically called ‘semicarbazones’. They are named in two ways:

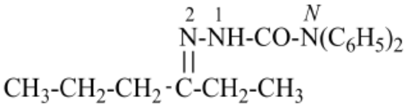
(1) substitutively by using the functional parent ‘hydrazinecarboxamide’;

(2) by the class modifier ‘semicarbazone’ placed after the name of the corresponding aldehyde or ketone.

Method (1) yields preferred IUPAC names.

Numerical locants are no longer used for the functional class name semicarbazone in preferred IUPAC names.

Example:



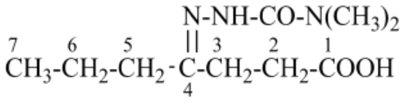
$$CH_3\text{-}CH_2\text{-}CH_2\text{-}\overset{\overset{2}{N}\text{-}\overset{1}{N}H\text{-}CO\text{-}\overset{\mathit{N}}{N}(C_6H_5)_2}{\overset{||}{C}}\text{-}CH_2\text{-}CH_3$$

2-(hexan-3-ylidene)-*N*,*N*-diphenylhydrazine-1-carboxamide (PIN)
2-(1-ethylbutylidene)-*N*,*N*-diphenylhydrazine-1-carboxamide
hexan-3-one 4,4-diphenylsemicarbazone

The compound prefix ‘carbamoylhydrazinylidene’ is used in the presence of a characteristic group that is preferred for citation as a suffix. This prefix is preferred to the traditional name ‘semicarbazono’, whose structure is numbered as follows:

$$=\overset{1}{N}\text{-}\overset{2}{N}H\text{-}\overset{3}{C}O\text{-}\overset{4}{N}H_2$$

Example:



$$\overset{7}{C}H_3\text{-}\overset{6}{C}H_2\text{-}\overset{5}{C}H_2\text{-}\underset{4}{\overset{N\text{-}NH\text{-}CO\text{-}N(CH_3)_2}{\overset{||}{C}}}\text{-}\overset{3}{C}H_2\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}OOH$$

4-[(dimethylcarbamoyl)hydrazinylidene]heptanoic acid (PIN)
4-(4,4-dimethylsemicarbazono)heptanoic acid

Chalcogen analogues of semicarbazones are named systematically as described for amides to give preferred IUPAC names, or by functional replacement nomenclature using the class terms ‘semicarbazone’ modified by the replacement prefixes ‘thio’, ‘seleno’, and ‘telluro’; for example, ‘thiosemicarbazone’. The prefix ‘carbamothioylhydrazinylidene’ is preferred to the traditional prefix ‘thiosemicarbazono’.

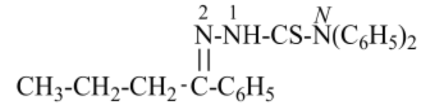
$$H_2\overset{2}{N}\text{-}\overset{1}{N}H\text{-}CS\text{-}\overset{\mathit{N}}{N}H_2$$

hydrazinecarbothioamide (PIN)

$$H_2\overset{1}{N}\text{-}\overset{2}{N}H\text{-}\overset{3}{C}S\text{-}\overset{4}{N}H_2$$

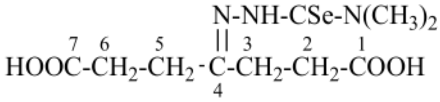
thiosemicarbazide

Examples:



$$\begin{array}{c}\overset{2}{N}\text{-}\overset{1}{N}H\text{-}CS\text{-}\overset{N}{N}(C_6H_5)_2\\ \| \\ CH_3\text{-}CH_2\text{-}CH_2\text{-}C\text{-}C_6H_5\end{array}$$

N,*N*-diphenyl-2-(1-phenylbutylidene)hydrazine-1-carbothioamide (PIN)
1-phenylbutan-1-one 4,4-diphenylthiosemicarbazone



$$\begin{array}{c}N\text{-}NH\text{-}CSe\text{-}N(CH_3)_2\\ \| \\ HOO\overset{7}{C}\text{-}\overset{6}{C}H_2\text{-}\overset{5}{C}H_2\text{-}\underset{4}{C}\text{-}\overset{3}{C}H_2\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}OOH\end{array}$$

4-[(dimethylcarbamoselenoyl)hydrazinylidene]heptanedioic acid (PIN)
4-[4,4-dimethyl(selenosemicarbazono)]heptanedioic acid

P-68.3.1.2.6 Hydrazinecarbohydrazide and derivatives

The preferred IUPAC name for the compound $H_2N\text{-}NH\text{-}CO\text{-}NH\text{-}NH_2$ is ‘hydrazinecarbohydrazide’. The name ‘carbonic dihydrazide’ is also recommended, but only for general nomenclature; the names ‘carbonohydrazide’, ‘carbohydrazide’, and ‘carbazide’ are not recommended. Systematic numbering is applied to the systematic name; a special numbering is assigned to carbonic dihydrazide, as follows:

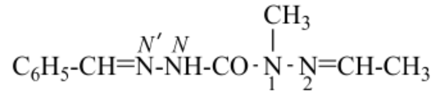
$$H_2\overset{2}{N}\text{-}\overset{1}{N}H\text{-}CO\text{-}\overset{N}{N}H\text{-}\overset{N'}{N}H_2$$

hydrazinecarbohydrazide (PIN)

$$H_2\overset{N'''}{N}\text{-}\overset{N''}{N}H\text{-}CO\text{-}\overset{N}{N}H\text{-}\overset{N'}{N}H_2$$

carbonic dihydrazide

Example:



$$\begin{array}{c}CH_3\\ | \\ C_6H_5\text{-}CH{=}\overset{N'}{N}\text{-}\overset{N}{N}H\text{-}CO\text{-}\underset{1}{N}\text{-}\underset{2}{N}{=}CH\text{-}CH_3\end{array}$$

N′-benzylidene-2-ethylidene-1-methylhydrazine-1-carbohydrazide (PIN)
(the twice substituted chain is the principal chain)
N‴-benzylidene-*N*′-ethylidene-*N*-methylcarbonic dihydrazide
(not *N*′-benzylidene-*N*‴-ethylidene-*N*″-methylcarbonic dihydrazide;
the set of locants ‘*N*,*N*′,*N*‴’ is lower than ‘*N*′,*N*″,*N*‴’)

As prefixes, the groups $–NH\text{-}NH\text{-}CO\text{-}NH\text{-}NH_2$ and $=N\text{-}NH\text{-}CO\text{-}NH\text{-}NH_2$ are called ‘hydrazinecarbohydrazido’ and ‘(hydrazinecarbonyl)hydrazinylidene’, respectively; these names are preferred prefixes.

Example:

$$H_2N\text{-}NH\text{-}CO\text{-}NH\text{-}NH\text{-}\overset{3}{C}H_2\text{-}CH_2\text{-}COOH$$

3-(hydrazinecarbohydrazido)propanoic acid (PIN)
3-[2-(hydrazinecarbonyl)hydrazin-1-yl]propanoic acid

P-68.3.1.3 Diazene and related compounds

P-68.3.1.3.1 Substitution of diazene
P-68.3.1.3.2 Azo compounds, R-N=N-R′
P-68.3.1.3.3 Azoxy compounds, R-N=N(O)-R′
P-68.3.1.3.4 Diazenecarbohydrazide, $HN{=}N\text{-}CO\text{-}NH\text{-}NH_2$
P-68.3.1.3.5 Formazan, $H_2N\text{-}N{=}CH\text{-}N{=}NH$
P-68.3.1.3.6 Carbodiazone [bis(diazenyl)methanone], HN=N-CO-N=NH
P-68.3.1.3.7 Isodiazene, $R_2N^+{=}N^–$

P-68.3.1.3.1 Substitution of diazene

Diazene is a modified parent hydride derived from the parent hydride diazane (see P-68.3.1.2.1) The prefix ‘diazenyl’ is a preselected prefix (see P-32.1.1).

Examples:

$$OHC\text{-}\overset{2}{N}{=}\overset{1}{N}\text{-}CHO$$

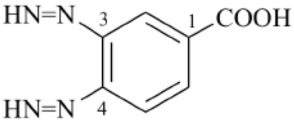
diazenedicarbaldehyde (PIN)

$$C_6H_5\text{-}\overset{2}{N}{=}\overset{1}{N}\text{-}CN$$

phenyldiazenecarbonitrile (PIN)

CH_3-N=N-CH_2-COOH
(methyldiazenyl)acetic acid (PIN)

HN=N-CH_2-CH_2-COOH
3-diazenylpropanoic acid (PIN)



3,4-bis(diazenyl)benzoic acid (PIN)

P-68.3.1.3.2 Azo compounds, R-N=N-R′

Note: Rules for naming azo compounds using the azo prefix were quite complex in the 1979 recommendations (ref. 1). Two sets of rules were recommended, the so-called 'old method' (Rule C-911) and the method used in CAS index nomenclature (Rule C-912) before 1972. The 'old method' (Rule C-911, ref. 1) must be totally discarded because some examples do not follow the basic rules developed in the 1979 organic nomenclature rules (ref. 1), especially with respect to the treatment of suffixes. In 1993, a new approach, introduced by CAS in 1972, was adopted based on the use of the parent hydride name 'diazene' [Method (1), below]. It brought simplicity and rationalization to the field and is the method chosen to generate preferred IUPAC names in these recommendations. However, names based on the method given as Rule C-912 in the 1979 recommendations are given here as an acceptable alternative for general nomenclature.

Compounds with the general structure R-N=N-R′, where R and R′ may be alike or different, are known generically as 'azo compounds'. They are named in two ways:

(1) substitutively using the parent 'diazene', HN=NH;

(2) by using the prefix 'azo' in the traditional manner (P-68.3.1.3.2.1).

Method (1) leads to preferred IUPAC names.

Azo compounds are divided into monoazo compounds, having one –N=N– group, bis(azo) compounds, having two –N=N– groups, and so on.

P-68.3.1.3.2.1 Symmetrical monoazo compounds, R-N=N-R, are named:

(1) by substituting the parent diazene, HN=NH, by the appropriate substituent groups;

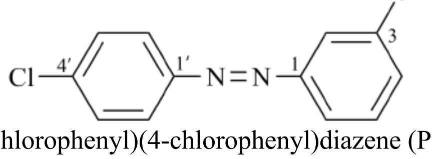
(2) by adding 'azo' to the name of the parent hydride, RH; substituents are denoted in the usual way by prefixes, the two RH parents being distinguished by unprimed and primed locants. Attachment of the azo group has priority for lowest available numbers.

Method (1) gives preferred IUPAC names.

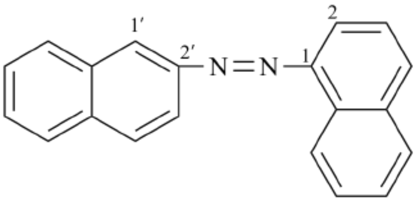
Examples:

CH_3-N=N-CH_3
dimethyldiazene (PIN)
azomethane

C_6H_5-N=N-C_6H_5
diphenyldiazene (PIN)
azobenzene



(3-chlorophenyl)(4-chlorophenyl)diazene (PIN)
3,4′-dichloroazobenzene (numbering shown)



(naphthalen-1-yl)(naphthalen-2-yl)diazene (PIN)
1,2′-azonaphthalene (numbering shown)

P-68.3.1.3.2.2 Unsymmetrical monoazo compounds are named in two ways:

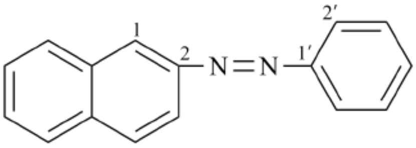
(1) substitutively, by prefixing the names of the appropriate substituent groups, in alphabetical order, before the parent hydride name diazene;

(2) by inserting 'azo' between the names of the parent hydrides RH and R′H; the principal chain or the senior ring or ring system is cited first and is assigned plain locants, the other parent hydride being given primed locants; when locants are required to denote the points of attachment of the parent hydrides, they are placed immediately before or after the prefix 'azo', respectively.

Method (1) leads to preferred IUPAC names.

Examples:

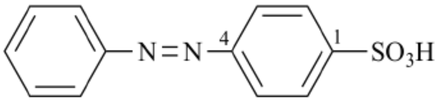
CH_2=CH-N=N-CH_3
ethenyl(methyl)diazene (PIN)
methyl(vinyl)diazene
etheneazomethane



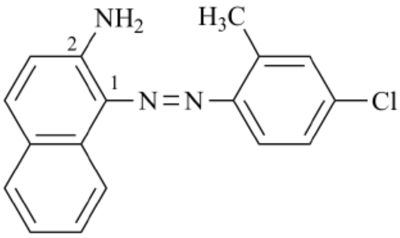
(naphthalen-2-yl)(phenyl)diazene (PIN)
naphthalene-2-azobenzene (numbering shown)

Monoazo compounds with the general structure R-N=N-R′ in which R is substituted by a principal characteristic group are named on the basis of the parent hydride, RH, substituted by an organyl diazenyl group, R′-N=N–. If both R and R′ are substituted by the same number of the principal characteristic group, a multiplicative name, using the prefix 'diazenediyl' for –N=N–, is preferred to a substitutive name.

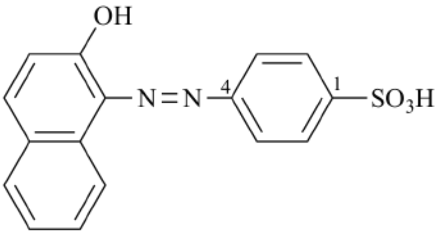
Examples:



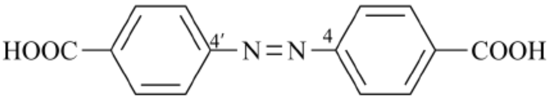
4-(phenyldiazenyl)benzene-1-sulfonic acid (PIN)



1-[(4-chloro-2-methylphenyl)diazenyl]naphthalen-2-amine (PIN)
[not 2-aminonaphthalene-1-azo(4′-chloro-2′-methylbenzene) (see C-911.2, ref. 1);
the principal characteristic group, the amine, must be denoted by a suffix]



4-[(2-hydroxynaphthalen-1-yl)diazenyl]benzene-1-sulfonic acid (PIN)
4-[(2-hydroxy-1-naphthyl)azo]benzene-1-sulfonic acid



4,4′-diazenediyldibenzoic acid (PIN)
(traditionally 4,4′-azodibenzoic acid)

P-68.3.1.3.2.3 Bis(azo) compounds and more complex analogues, in the absence of a characteristic group having seniority to be cited as suffix, are named:

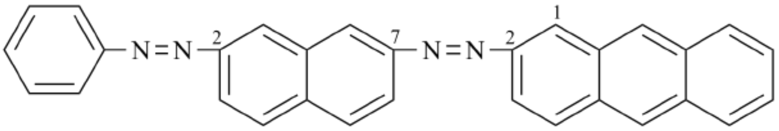
(1) on the basis of 'diazene', as described in P-68.3.1.3.2.1 above, the first cited substituent being chosen on the basis of the principle of alphanumerical order;

(2) by using the prefix 'azo', as described in P-68.3.1.3.2.1;

(3) by using the prefix 'azo' and, after choosing the principal parent hydride, substituting the other components as an 'organylazo' group.

Method (1) generates preferred IUPAC names.

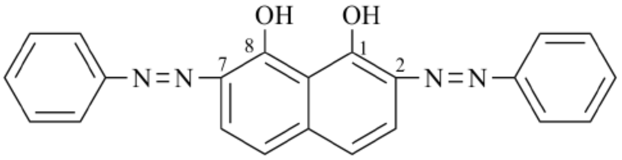
Example:



(1) {7-[(anthracen-2-yl)diazenyl]naphthalen-2-yl}(phenyl)diazene(PIN)
{not (anthracen-2-yl)[7-(phenyldiazenyl)naphthalen-2-yl]diazene;
each primary substituent has the same locant, i.e., none,
so 'anthracenyldiazenyl' is alphabtically preferred to 'anthracenylphenyl'}
(2) anthracene-2-azo-2′-naphthalene-7′-azobenzene)
(3) 2-{[7-(phenylazo)naphthalen-2-yl]azo}anthracene

When characteristic groups that have priority for citation as suffixes are present, the usual substitutive operations based on priority of suffixes are carried out. Names based on the prefix 'diazenyl' are preferred to those using 'azo' for generating preferred IUPAC names.

Example:



2,7-bis(phenyldiazenyl)naphthalene-1,8-diol (PIN)
2,7-bis(phenylazo)naphthalene-1,8-diol

P-68.3.1.3.3 Azoxycompounds, R-N=N(O)-R′

P-68.3.1.3.3.1 *N*-Oxides of azo compounds having the general structure R-N_2(O)-R′ (R = R′ or R ≠ R′) are known generically as 'azoxy compounds'. Their nomenclature was revised in 1993 (ref. 2) and is used in these recommendations. Azoxy compounds are named in two different ways:

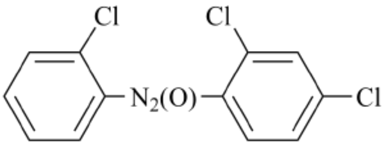
(1) by adding the term 'oxide' to the name of the corresponding azo compound, preceded by a locant 1 or 2;

(2) in the traditional way of replacing the prefix 'azo' by 'azoxy' and using the locants *NNO* and *ONN* to indicate the parent hydride associated with the =N(O) group. In the general structure R-N(O)N-R′, the symbol *NNO* specifies that the oxygen atom is attached to the nitrogen atom next to the R′ group. The symbol *ONN* specifies that the oxygen atom is attached to the nitrogen atom next to the R group. When the point of attachment is not known, the symbol *NON* is used.

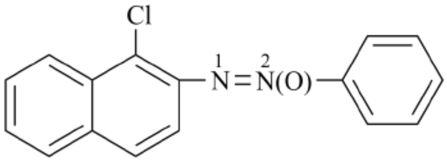
Method (1) leads to preferred IUPAC names. Azoxy compounds could also be named by using the λ-convention or as zwitterions.

Examples:

C_6H_5-N=N(O)-C_6H_5
(1) diphenyldiazene oxide (PIN)
(2) azoxybenzene
1-oxo-1,2-diphenyl-1λ^5-diazene (see P-74.2.2.1.4)
(diphenyldiazeniumyl)oxidanide (see P-74.2.2.1.4)



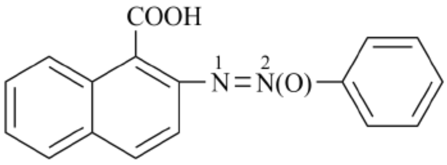
(2-chlorophenyl)(2,4-dichlorophenyl)diazene oxide (PIN)
(the absence of locants indicates that the points of attachment are not known)
2,2′,4-trichloroazoxybenzene



1-(1-chloronaphthalen-2-yl)-2-phenyldiazene 2-oxide (PIN)
1-chloro-2-(phenyl-*ONN*-azoxy)naphthalene

P-68.3.1.3.3.2 An azoxy compound, according to the general seniority given to zwitterions over suffixes expressing characteristic groups, is preferably named as a derivative of diazene oxide, unless some other priority is given to another radical or ionic group. In general nomenclature, the traditional method for naming azoxy compounds is maintained. An azoxy compound in which the general structure is R-N=N(O)-R′ or R′-N=N(O)-R, in which R is substituted by a principal characteristic group is named on the basis of the parent hydride, RH, substituted by the R′-azoxy group in which the position of the oxygen atom is denoted by the prefix *NNO*-, *ONN*-, or *NON*-, as appropriate.

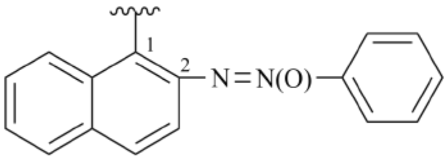
Example:



1-(1-carboxynaphthalen-2-yl)-2-phenyldiazene 2-oxide (PIN)
2-(phenyl-*ONN*-azoxy)naphthalene-1-carboxylic acid
[not 2-(phenyl-*ONN*-azoxy)-1-naphthoic acid;
no substitution allowed on naphthoic acid]

When the azoxy compound has to be expressed by a prefix, substitutive nomenclature using the λ-convention is preferred (see P-14.1).

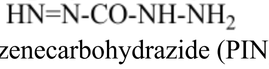
Example:



2-(2-phenyl-2-oxo-2λ^5-diazenyl)naphthalen-1-yl (preferred prefix)
2-(2-oxido-2-phenyldiazen-2-ium-1-yl)naphthalen-1-yl

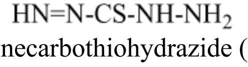
P-68.3.1.3.4 Diazenecarbohydrazide, $HN=N\text{-}CO\text{-}NH\text{-}NH_2$

The hydrazide of 'diazenecarboxylic acid', $HN=N\text{-}CO\text{-}NH\text{-}NH_2$, is named systematically 'diazenecarbohydrazide'; it is the preferred IUPAC name. The name 'carbazone' is not recommended. Chalcogen analogues are named by using the infixes and the prefixes 'thio', 'seleno', and 'telluro'.



$H\overset{2}{N}=\overset{1}{N}\text{-CO-}\overset{N}{N}H\text{-}\overset{N'}{N}H_2$

diazenecarbohydrazide (PIN)

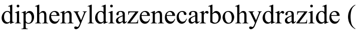


$H\overset{2}{N}=\overset{1}{N}\text{-CS-}\overset{N}{N}H\text{-}\overset{N'}{N}H_2$

diazenecarbothiohydrazide (PIN)

Note: Numerical locants that were used for the name 'carbazone' that is now abandoned are not transferred to the preferred IUPAC name 'diazenecarbohydrazide'.

Examples:



$C_6H_5\text{-}\overset{2}{N}=\overset{1}{N}\text{-CO-}\overset{N}{N}H\text{-}\overset{N'}{N}H\text{-}C_6H_5$

N′,2-diphenyldiazenecarbohydrazide (PIN)

$C_6H_5\text{-}\overset{2}{N}{=}\overset{1}{N}\text{-}CS\text{-}\overset{N}{N}H\text{-}\overset{N'}{N}H\text{-}C_6H_5$

N′,2-diphenyldiazenecarbothiohydrazide (PIN)

As a prefix, the group –HN-NH-CO-N=NH is named ‘2-(diazenecarbonyl)hydrazin-1-yl’ or ‘diazenecarbohydrazido’ (preferred prefix). The name ‘carbazono’ is not recommended.

The group $H_2N\text{-}NH\text{-}CO\text{-}N{=}N\text{–}$ is named ‘(hydrazinecarbonyl)diazenyl’.

Example:

$HN{=}N\text{-}CO\text{-}NH\text{-}NH\text{-}CH_2\text{-}CH_2\text{-}COO\text{-}CH_2\text{-}CH_3$

ethyl 3-(diazenecarbohydrazido)propanoate (PIN)

ethyl 3-[2-(diazenecarbonyl)hydrazin-1-yl]propanoate

P-68.3.1.3.5 Formazan, $H_2N\text{-}N{=}CH\text{-}N{=}NH$

The hydrazone of diazenecarbaldehyde, $H_2N\text{-}N{=}CH\text{-}N{=}NH$, has the retained name, which is also the preferred IUPAC name ‘formazan’; it is numbered in a special manner. It can also be named substitutively as a derivative of the parent hydride ‘hydrazine’; its derivatives are named accordingly.

$H_2\overset{5}{N}\text{-}\overset{4}{N}{=}\overset{3}{C}H\text{-}\overset{2}{N}{=}\overset{1}{N}H$

formazan (PIN)

$H_2\overset{2}{N}\text{-}\overset{1}{N}{=}CH\text{-}N{=}NH$

(diazenylmethylidene)hydrazine

P-68.3.1.3.5.1 Derivatives of formazan

Preferred names are constructed systematically as derivatives of formazan when prefixes only are present or when the principal characteristic group is attached directly to the formazan structure. Otherwise, the functionalized formazan parent must be expressed according to the seniority rules applied in constructing names (see P-4).

Examples:

$H_2\overset{5}{N}\text{-}\overset{4}{N}{=}\overset{3}{C}(C_6H_5)\text{-}\overset{2}{N}{=}\overset{1}{N}\text{-}C_6H_5$

1,3-diphenylformazan (PIN)

[phenyl(phenyldiazenyl)methylidene]hydrazine

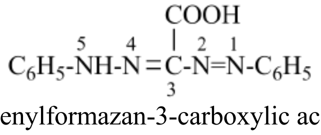
phenyl(phenyldiazenyl)methanone hydrazone

$C_6H_5\text{-}\overset{5}{N}H\text{-}\overset{4}{N}{=}\overset{3}{C}(C_6H_5)\text{-}\overset{2}{N}{=}\overset{1}{N}H$

3,5-diphenylformazan (PIN)

[diazenyl(phenyl)methylidene]phenylhydrazine

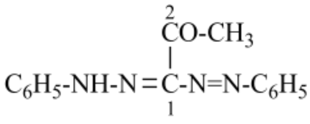
phenyl(diazenyl)methanone 2-phenylhydrazone



$C_6H_5\text{-}\overset{5}{N}H\text{-}\overset{4}{N}{=}\underset{3}{\overset{COOH}{C}}\text{-}\overset{2}{N}{=}\overset{1}{N}\text{-}C_6H_5$

1,5-diphenylformazan-3-carboxylic acid (PIN)

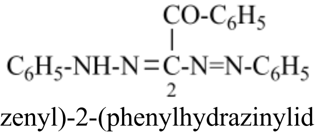
(phenyldiazenyl)(phenylhydrazinylidene)acetic acid



$C_6H_5\text{-}NH\text{-}N{=}\underset{1}{\overset{\overset{2}{C}O\text{-}CH_3}{C}}\text{-}N{=}N\text{-}C_6H_5$

1-(phenyldiazenyl)-1-(phenylhydrazinylidene)propan-2-one (PIN)

3-acetyl-1,5-diphenylformazan



$C_6H_5\text{-}NH\text{-}N{=}\underset{2}{\overset{\overset{1}{C}O\text{-}C_6H_5}{C}}\text{-}N{=}N\text{-}C_6H_5$

1-phenyl-2-(phenyldiazenyl)-2-(phenylhydrazinylidene)ethan-1-one (PIN)

3-benzoyl-1,5-diphenylformazan

$CH_3\text{-}CO\text{-}\overset{N}{N}H\text{-}\overset{N'}{N}{=}CH\text{-}N{=}N\text{-}C_6H_5$

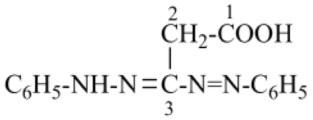
N′-[(phenyldiazenyl)methylidene]acetohydrazide (PIN)

P-68.3.1.3.5.2 Prefixes derived from formazan for substitutive nomenclature

Substituent groups derived from formazan are as follows; retained names lead to preferred IUPAC prefixes.

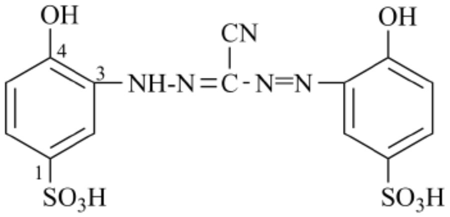
	Preferred prefix	**Systematic prefix**
$\mathrm{H_2\overset{5}{N}\text{-}\overset{4}{N}{=}\overset{3}{C}H\text{-}\overset{2}{N}{=}\overset{1}{N}\text{–}}$	formazan-1-yl	(hydrazinylidenemethyl)diazenyl
$\mathrm{H\overset{1}{N}{=}\overset{2}{N}\text{-}\overset{3}{C}H{=}\overset{4}{N}\text{-}\overset{5}{N}H\text{–}}$	formazan-5-yl	(diazenylmethylidene)hydrazinyl
$\mathrm{H_2\overset{5}{N}\text{-}\overset{4}{N}{=}\underset{3}{\overset{\vert}{C}}\text{-}\overset{2}{N}{=}NH}$	formazan-3-yl	diazenyl(hydrazinylidene)methyl
$\mathrm{\text{–}H\overset{5}{N}\text{-}\overset{4}{N}{=}\overset{3}{C}H\text{-}\overset{2}{N}{=}N\text{–}}$	formazan-1,5-diyl	
$\mathrm{H\overset{1}{N}{=}\overset{2}{N}\text{-}\underset{3}{\overset{\vert}{C}}{=}\overset{4}{N}\text{-}\overset{5}{N}H\text{–}}$	formazan-3,5-diyl	
$\mathrm{{=}\overset{5}{N}\text{-}\overset{4}{N}{=}\overset{3}{C}H\text{-}\overset{2}{N}{=}\overset{1}{N}\text{–}}$	formazan-1-yl-5-ylidene	
$\mathrm{{=}\overset{5}{N}\text{-}\overset{4}{N}{=}\underset{3}{\overset{\vert}{C}}\text{-}\overset{2}{N}{=}\overset{1}{N}H}$	formazan-3-yl-5-ylidene	
$\mathrm{\text{–}\overset{5}{N}H\text{-}\overset{4}{N}{=}\underset{3}{\overset{\vert}{C}}\text{-}\overset{2}{N}{=}\overset{1}{N}\text{–}}$	formazan-1,3,5-triyl	

Examples:



$$\mathrm{C_6H_5\text{-}NH\text{-}N{=}\underset{3}{\overset{\overset{2}{C}H_2\text{-}\overset{1}{C}OOH}{\vert}}{C}\text{-}N{=}N\text{-}C_6H_5}$$

3-(phenyldiazenyl)-3-(phenylhydrazinylidene)propanoic acid (PIN;
propanoic acid is preferred to acetic acid)
(1,5-diphenylformazan-3-yl)acetic acid



3,3′-(3-cyanoformazan-1,5-diyl)bis(4-hydroxybenzene-1-sulfonic acid) (PIN)
3-(2-{cyano[(2-hydroxy-5-sulfophenyl)diazenyl]methylidene}hydrazinyl)-4-hydroxybenzene-1-sulfonic acid
{not 3-({cyano[(2-hydroxy-5-sulfophenyl)hydrazinylidene]methyl}diazenyl)-4-hydroxybenzene-1-sulfonic acid
('cyanohydroxysulfophenyldiazenyl...' is lower alphabetically than 'cyanohydroxysulfophenylhydrazinylidene...'}

P-68.3.1.3.6 Carbodiazone [bis(diazenyl)methanone], HN=N-CO-N=NH

The compound HN=N-CO-N=NH is named systematically bis(diazenyl)methanone; its hydrocarbyl derivatives are named substitutively. Such names are preferred IUPAC names over those denoted by the retained name 'carbodiazone', which can be used in general nomenclature with full substitution according to a special numbering. The name 'bis(diazenyl)methanone' is preferred to 1,1′-carbonylbis(diazene) simply because a ketone, expressed by the suffix 'one', is senior to the parent structure 'diazane' or 'diazene' (see P-41).

Chalcogen analogues of bis(diazenyl)methanone are also named systematically as bis(diazenyl)methanethione, -selone, and -tellone, respectively. The prefixes thio, seleno, and telluro are used with the name carbodiazone in general nomenclature.

Examples:

HN=N-CO-N=NH
bis(diazenyl)methanone (PIN)
[not 1,1′-carbonylbis(diazene)]

$\mathrm{H\overset{1}{N}{=}\overset{2}{N}\text{-}\overset{3}{C}O\text{-}\overset{4}{N}{=}\overset{5}{N}H}$
carbodiazone

HN=N-CS-N=NH
bis(diazenyl)methanethione (PIN)
thiocarbodiazone

HN=N-CO-N=N–
(diazenecarbonyl)diazenyl (preferred prefix)

$C_6H_5\text{-}N{=}N\text{-}CO\text{-}N{=}N\text{-}C_6H_5$
bis(phenyldiazenyl)methanone (PIN)
1,5-diphenylcarbodiazone

P-68.3.1.3.7 Isodiazenes, $R_2N^+{=}N^-$

Compounds with the general structure $R_2N\text{-}N{:}$ ↔ $R_2N^+{=}N^-$ are called 'isodiazenes' generically and are named substitutively on the basis of the parent radical 'hydrazinylidene', $H_2N\text{-}N{:}$. This method leads to preferred IUPAC names rather than the names based on the parent hydride name 'isodiazene'.

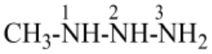
Example:

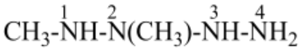
$(CH_3)_2N\text{-}N{:}$
dimethylhydrazinylidene (PIN)
dimethylisodiazene

P-68.3.1.4 Polyazanes

P-68.3.1.4.1 Acyclic polyazanes are saturated chains of nitrogen atoms; hydrazine is the retained name and the preselected name for diazane, $H_2N\text{-}NH_2$. Names are formed by prefixing the mononuclear parent hydride name 'azane' with an appropriate numerical prefix and numbered in the same way as hydrocarbons. The parent hydrides are preselected names (see P-12.2). The final 'a' of a numerical prefix is not elided before 'azane'.

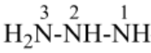
Examples:

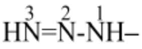

$CH_3\text{-}\overset{1}{N}H\text{-}\overset{2}{N}H\text{-}\overset{3}{N}H_2$
1-methyltriazane. (PIN)


$CH_3\text{-}\overset{1}{N}H\text{-}\overset{2}{N}(CH_3)\text{-}\overset{3}{N}H\text{-}\overset{4}{N}H_2$
1,2-dimethyltetraazane (PIN)

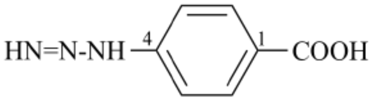
The corresponding prefixes are named according to the general method described in P-29. The traditional names 'triazano' and 'triazeno', now called epitriazano and epitriazeno (see P-25.4.2.1.4), are names of bridges in bridged fused ring names and must not be used as substituent group names.

> The formation of systematic prefix names, i.e., triazan-1-yl, etc., as described in P-29, must be considered a change even though the names triazano, tetrazano, etc., previously used as names for bridges in the naming of bridge fused ring systems, are no longer used as such and have been replaced by the names 'epitriazano', etc. (see P-25.4.2.1.4).

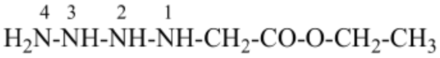

$H_2\overset{3}{N}\text{-}\overset{2}{N}H\text{-}\overset{1}{N}H–$
triazan-1-yl (preselected prefix)
(not triazano)


$H\overset{3}{N}{=}\overset{2}{N}\text{-}\overset{1}{N}H–$
triaz-2-en-1-yl (preselected prefix)
(not triaz-2-eno)

Examples:



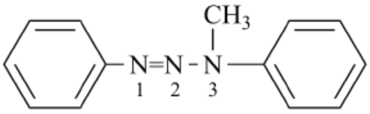
4-(triaz-2-en-1-yl)benzoic acid (PIN)
[not 4-(triaz-2-eno)benzoic acid]


$H_2\overset{4}{N}\text{-}\overset{3}{N}H\text{-}\overset{2}{N}H\text{-}\overset{1}{N}H\text{-}CH_2\text{-}CO\text{-}O\text{-}CH_2\text{-}CH_3$
ethyl (tetraazan-1-yl)acetate (PIN)
[not ethyl tetrazanoacetate)

P-68.3.1.4.2 Diazoamino compounds

Compounds having the structure $R\text{-}N{=}N\text{-}NR_2$ are known as 'diazoamino compounds' when the same substituent group is located at each end of the chain. They are named substitutively, on the basis of the parent hydride name 'triazene' if there is present no characteristic group to be cited as a suffix. The prefix 'diazoamino' for the group –N=N-NH– is no longer recommended.

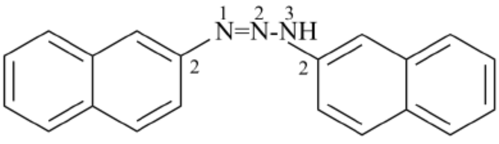
Examples:



3-methyl-1,3-diphenyltriaz-1-ene (PIN)
(formerly *N*-methyldiazoaminobenzene)

$$C_6H_5\text{-}\overset{1}{N}{=}\overset{2}{N}\text{-}\overset{3}{N}H\text{-}C_6H_5$$

1,3-diphenyltriaz-1-ene (PIN)
(formerly diazoaminobenzene)



1,3-di(naphthalen-2-yl)triaz-1-ene (PIN)
(formerly 2,2′-diazoaminonaphthalene)

P-68.3.2 Phosphorus, arsenic, and antimony compounds

P-68.3.2.1 General methodology

Preferred names of acyclic phosphorus, arsenic, and antimony compounds are functional class names (see P-67) derived from mononuclear and polynuclear acids, such as phosphoric acid, H_3PO_4, arsonous acid, $HAs(OH)_2$, stibinic acid, $H_2Sb(O)(OH)$, and diphosphonic acid, HO-HP(O)-O-P(O)H-OH, rather than substitutive names based on parent hydrides.

Other preferred names of acyclic and cyclic compounds are substitutive names, in accordance with the seniority of classes (see P-41).

This subsection includes the description of functional class nomenclature and substitutive nomenclature.

P-68.3.2.2 Parent hydrides
P-68.3.2.3 Substitutive nomenclature

P-68.3.2.2 Parent hydrides

Parent hydrides are formed by the methods described in Chapter P-2. They are mononuclear, acyclic polynuclear, and cyclic ring systems and are preselected names (see P-12.2) The λ-convention is used to denote pentavalent phosphorus and arsenic atoms. Retained names for use only in general nomenclature are phosphine, phosphorane, arsine, arsorane, stibine, and stiborane.

Preferred names are selected as indicated in Chapter P-2.

Examples:

PH_3
phosphane (preselected name)
phosphine

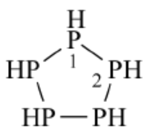
AsH_5
λ^5-arsane (preselected name)
arsorane

$$H_2\overset{2}{P}\text{-}\overset{1}{P}H_2$$

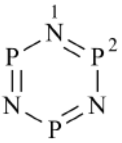
diphosphane (preselected name)
diphosphine

$$H_2\overset{5}{As}\text{-}\overset{4}{As}H\text{-}\overset{3}{As}H\text{-}\overset{2}{As}H\text{-}\overset{1}{As}H_2$$

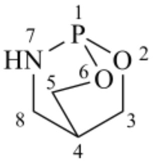
pentaarsane (preselected name)



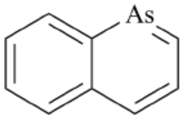
pentaphospholane (preselected name)
cyclopentaphosphane



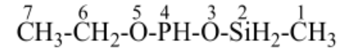
1,3,5,2,4,6-triazatriphosphinine (preselected name)
(not cyclotriphosphazene, which has only one double bond)



2,6-dioxa-7-aza-1-phosphabicyclo[2.2.2]octane (PIN)

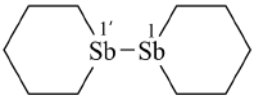


arsinoline (PIN)



$$\overset{7}{C}H_3\text{-}\overset{6}{C}H_2\text{-}\overset{5}{O}\text{-}\overset{4}{P}H\text{-}\overset{3}{O}\text{-}\overset{2}{Si}H_2\text{-}\overset{1}{C}H_3$$

ethyl methylsilyl phosphonite (PIN)
3,5-dioxa-4-phospha-2-silaheptane



1,1′-bistibinane (PIN)

P-68.3.2.3 Substitutive nomenclature

Compounds not named in accordance with the previous section, P-68.3.2.2 are named substitutively on the basis of acyclic and cyclic parent hydrides, using suffixes and prefixes to designate characteristic groups.

P-68.3.2.3.1 Substitutive nomenclature, suffix mode

Suffixes are used to denote characteristic groups present as principal groups, with the exception of acids having retained names and their derivatives, as described in P-67. This method produces preferred IUPAC names over those formed by functional class nomenclature, where =O, =S, =Se, =Te, =NH are denoted by the class names oxide, sulfide, selenide, telluride, and imide added to the name of the parent hydride.

Examples:

$H_2P\text{-}COOH$
phosphanecarboxylic acid (PIN)

$H_2P\text{-}CO\text{-}NH_2$
phosphanecarboxamide (PIN)

$C_6H_5\text{-}P{=}O$
phenylphosphanone (PIN)
[not oxo(phenyl)phosphane]

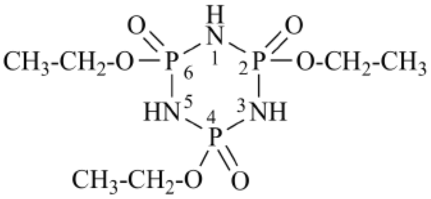
$(C_6H_5)_3P{=}O$
triphenyl-λ^5-phosphanone (PIN)
triphenylphosphane oxide
(not oxotriphenyl-λ^5-phosphane)

$HP{=}N\text{-}CH_3$
N-methylphosphanimine (PIN)
[not (methylimino)phosphane]

$(CH_3)_3As{=}Te$
trimethyl-λ^5-arsanetellone (PIN)
trimethylarsane telluride

$C_6H_5\text{-}As{=}S$
phenylarsanethione (PIN)
[not phenyl(sulfanylidene)arsane]

$(CH_3)_3As{=}NH$
As,*As*,*As*-trimethyl-λ^5-arsanimine (PIN)
trimethylarsane imide



2,4,6-triethoxy-1,3,5,2λ^5,4λ^5,6λ^5-triazatriphosphinane-2,4,6-trione (PIN)

P-68.3.2.3.2 Substitutive nomenclature, prefix mode

The seniority of classes must be applied in the following order: classes expressed by suffixes, then classes in order of the heteroatom class, i.e., N > P > As > Sb > Bi > Si > Ge > Sn > Pb > B > Al > Ga > In > Tl > O > S > Se > and Te.

P-68.3.2.3.2.1 Substitution of phosphanes, arsanes, and stibanes by organyl groups

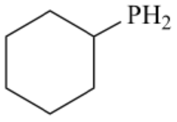
Alkyl, aryl, etc. groups and groups derived from parent hydrides containing O, S, Se, and Te atoms are always denoted by prefixes. Halides and pseudohalides are not expressed by prefixes when attached directly to a P, As, or Sb atom, because functional replacement of parent acids having retained names is senior for naming them as acid halides or pseudohalides (see P-67.1.2.5.1).

Examples:

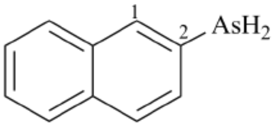
$(C_6H_5)_3P$
triphenylphosphane (PIN)
triphenylphosphine

$CH_3\text{-}CH_2\text{-}AsH_2$
ethylarsane (PIN)
ethylarsine

$P(OCH_3)_5$
pentamethoxy-λ^5-phosphane (PIN)

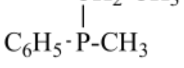


cyclohexylphosphane (PIN)
cyclohexylphosphine



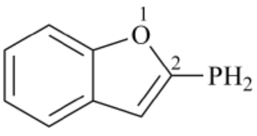
(naphthalen-2-yl)arsane (PIN)
(naphthalen-2-yl)arsine
2-naphthylarsane

$ClCH_2\text{-}CH_2\text{-}AsH\text{-}CHCl\text{-}CH_3$
(1-chloroethyl)(2-chloroethyl)arsane (PIN)
(1-chloroethyl)(2-chloroethyl)arsine

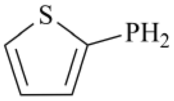


$$C_6H_5\text{-}\overset{\displaystyle CH_2\text{-}CH_3}{\overset{|}{P}}\text{-}CH_3$$

ethyl(methyl)(phenyl)phosphane (PIN)
ethyl(methyl)(phenyl)phosphine

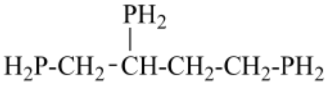


(1-benzofuran-2-yl)phosphane (PIN)
(1-benzofuran-2-yl)phosphine



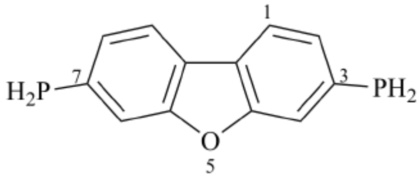
(thiophen-2-yl)phosphane (PIN)
(thiophen-2-yl)phosphine

$(CH_3)_2P\text{-}CH_2\text{-}CH_2\text{-}P(CH_3)_2$
(ethane-1,2-diyl)bis(dimethylphosphane) (PIN)
(ethane-1,2-diyl)bis(dimethylphosphine)

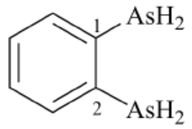


$H_2P\text{-}CH_2\text{-}\overset{\overset{\displaystyle PH_2}{|}}{C}H\text{-}CH_2\text{-}CH_2\text{-}PH_2$

(butane-1,2,4-triyl)tris(phosphane) (PIN)
(butane-1,2,4-triyl)tris(phosphine)



(dibenzo[*b*,*d*]furan-3,7-diyl)bis(phosphane) (PIN)
(dibenzofuran-3,7-diyl)bis(phosphine)



(1,2-phenylene)bis(arsane) (PIN)
(1,2-phenylene)bis(arsine)

P-68.3.2.3.2.2 Phosphanes, arsanes, and stibanes expressed as substituent groups

Substituent groups are formed by the general method described in Section P-29, i.e., by adding the suffixes ‘yl’, ‘ylidene’ and ‘ylidyne’ to the name of the parent hydride with elision of the final letter ‘e’ of the parent hydride name. When required, the order of classes is applied, as indicated in Section P-41. The traditional names phosphino, arsino, and stibino may be used in general nomenclature.

$–PH_2$
phosphanyl (preselected prefix)
phosphino

–As=
arsanylylidene (preselected prefix)

–HP-PH–
diphosphane-1,2-diyl (preselected prefix)

–As<
arsanetriyl (preselected prefix)

$–AsH_2$
arsanyl (preselected prefix)
arsino

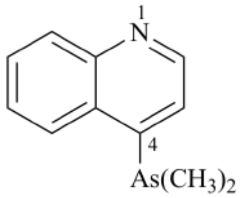
$–SbH_2$
stibanyl (preselected prefix)
stibino

$–SbH\text{-}SbH_2$
distibanyl (preselected prefix)

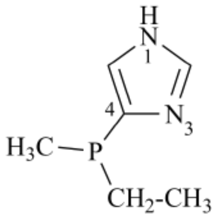
Examples:

$H_2P\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}H_2\text{-}NH_2$
2-phosphanylethan-1-amine (PIN)
2-phosphinoethan-1-amine

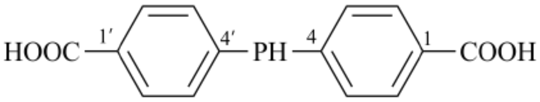
$H_2As\text{-}CH_2\text{-}P(C_6H_5)_2$
(arsanylmethyl)di(phenyl)phosphane (PIN)
(arsinomethyl)di(phenyl)phosphine



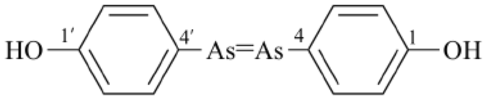
4-(dimethylarsanyl)quinoline (PIN)
4-(dimethylarsino)quinoline


H
N
1
4
N3
H3C
P
CH2-CH3

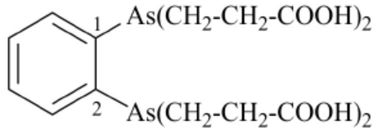
4-[ethyl(methyl)phosphanyl]-1*H*-imidazole (PIN)
4-[ethyl(methyl)phosphino]-1*H*-imidazole


HOOC
1′
4′
PH
4
1
COOH

4,4′-phosphanediyldibenzoic acid (PIN)

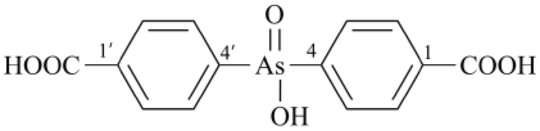

HO
1′
4′
As=As
4
1
OH

4,4′-diarsenediyldiphenol (PIN)

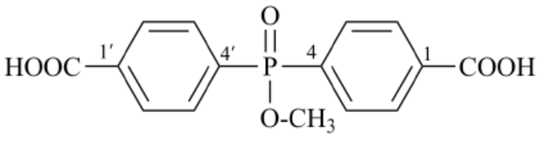

1
As(CH2-CH2-COOH)2
2
As(CH2-CH2-COOH)2

3,3′,3″,3‴-[1,2-phenylenebis(arsanetriyl)]tetrapropanoic acid (PIN)

$(HO)_2As(O)\text{-}CH_2\text{-}COOH$
arsonoacetic acid (PIN)


O
HOOC
1′
4′
As
4
1
COOH
OH

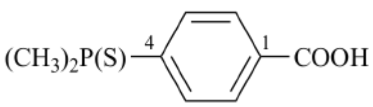
4,4′-(hydroxyarsoryl)dibenzoic acid (PIN)
(not 4,4′-arsinicodibenzoic acid)


O
HOOC
1′
4′
P
4
1
COOH
O-CH3

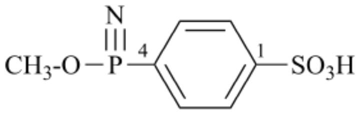
4,4′-(methoxyphosphoryl)dibenzoic acid (PIN)

$Cl_2P(O)\text{-}CH_2\text{-}CO\text{-}Cl$
phosphorodichloridoylacetyl chloride (PIN)
(dichlorophosphoryl)acetyl chloride

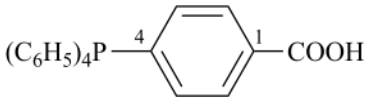
$(CH_3O)_2P(=NH)\text{-}CH_2\text{-}CO\text{-}O\text{-}CH_3$
methyl (*P*,*P*-dimethoxyphosphinimidoyl)acetate (PIN)


(CH3)2P(S)
4
1
COOH

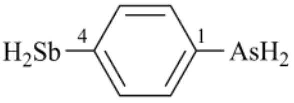
4-(dimethylphosphinothioyl)benzoic acid (PIN)



4-(methoxyphosphoronitridoyl)benzene-1-sulfonic acid (PIN)



4-(tetraphenyl-λ^5-phosphanyl)benzoic acid (PIN)
4-(tetraphenylphosphoranyl)benzoic acid



(4-stibanylphenyl)arsane (PIN)
(4-stibinophenyl)arsine

P-68.3.3 Bismuth compounds

Bismuth compounds are named substitutively on the basis of parent hydrides named in accordance with the rules described in Chapter P-2. Suffixes and prefixes are used as indicated for substitutive nomenclature. There are no acids having retained names subject to functional class nomenclature. Substitutive nomenclature is preferred to functional nomenclature to designate oxides, sulfides, selenides, tellurides, and imides. Preferred and preselected names are chosen as for P, As, and Sb parents and prefixes.

BiH_3
bismuthane (preselected name)
bismuthine

BiH_5
λ^5-bismuthane (preselected name)
bismuthorane

$H_2Bi\text{-}BiH_2$
dibismuthane (preselected name)

$H_2Bi–$
bismuthanyl (preselected prefix)
bismuthino

$H_3Bi=$
λ^5-bismuthanylidene (preselected prefix)

$–HBi\text{-}BiH–$
dibismuthane-1,2-diyl (preselected prefix)

Examples:

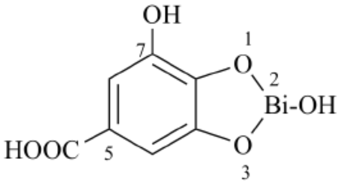
$Bi(CH{=}CH_2)_3$
triethenylbismuthane (PIN)
trivinylbismuthine

$Bi(CH_3)_3$
trimethylbismuthane (PIN)
trimethylbismuthine

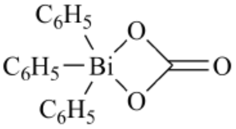
$(C_6H_5)_3Bi{=}O$
triphenyl-λ^5-bismuthanone (PIN)
triphenylbismuthane oxide

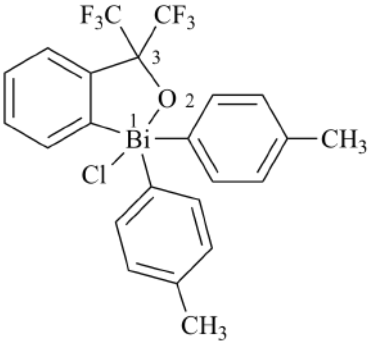
$(C_6H_5)_3Bi{=}NH$
Bi.Bi,*Bi*-triphenyl-λ^5-bismuthanimine (PIN)
triphenylbismuthane imide

$O{=}\overset{5}{Bi}\text{-}\overset{4}{O}\text{-}\overset{3}{C}O\text{-}\overset{2}{O}\text{-}\overset{1}{Bi}{=}O$
bis(oxobismuthanyl) carbonate (PIN)
2,4-dioxa-1,5-dibismapentane-1,3,5-trione


2,7-dihydroxy-2*H*-1,3,2-benzodioxabismole-5-carboxylic acid (PIN)

$(C_6H_5)_3BiCl_2$
dichlorotri(phenyl)-λ^5-bismuthane (PIN)
dichlorotri(phenyl)bismuthorane


2,2,2-triphenyl-1,3,2λ^5-dioxabismetan-4-one (PIN)


1-chloro-1,1-bis(4-methylphenyl)-3,3-bis(trifluoromethyl)-1,3-dihydro-2,1λ^5-benzoxabismole (PIN)

P-68.4 NOMENCLATURE FOR COMPOUNDS OF THE GROUP 16 ELEMENTS

P-68.4.0 Introduction
P-68.4.1 Three or more homogeneous contiguous chalcogen atoms
P-68.4.2 Three or more heterogeneous contiguous chalcogen atoms
P-68.4.3 Chalcogen parent hydrides with nonstandard bonding numbers

P-68.4.0 Introduction

The nomenclature of compounds containing chalcogen atoms depends on the number and kind of chalcogen atoms present. When one or two contiguous chalcogen atoms are present, chalcogen atoms are not used as parent hydrides, except for sulfones and disulfones when they are able to be expressed as described in previous sections. Hydroxy compounds, ethers, peroxols, peroxides, and their chalcogen analogues are described in P-63. However, when three or more contiguous identical chalcogen atoms are present these chalcogen atoms are always treated as parent hydrides in the normal way.

Sulfoxides and sulfones are also included in this type of nomenclature (see P-63.6).

P-68.4.1 Three or more homogeneous contiguous chalcogen atoms

P-68.4.1.1 Compounds with three or more contiguous identical chalcogen atoms are treated as parent hydrides in substitutive nomenclature.

Examples:

HO-O-OH
trioxidane (preselected name)

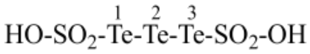
CH_3-S-S-SH
methyltrisulfane (PIN)

CH_3-O-O-O-CH_3
dimethyltrioxidane (PIN)
dimethyl trioxide

CH_3-S-S-S-CH_3
dimethyltrisulfane (PIN)
dimethyl trisulfide

C_6H_5-Se-Se-Se-CH_3
methyl(phenyl)triselane (PIN)
methyl phenyl triselenide

C_6H_5-Se-Se-Se-C_6H_5
diphenyltriselane (PIN)
diphenyl triselenide
(not triselanediyldibenzene)


$HO\text{-}SO_2\text{-}\overset{1}{Te}\text{-}\overset{2}{Te}\text{-}\overset{3}{Te}\text{-}SO_2\text{-}OH$
tritellanedisulfonic acid (preselected name)
tritelluropentathionic acid (traditional name)

HO-SO_2-S-S-S-SO_2-OH
trisulfanedisulfonic acid (preselected name)
pentathionic acid (traditional name)

CH_3-SeSeSe-O-SH
methyltriselane-*OS*-thioperoxol (PIN)
O-(methyltriselanyl) thiohydroperoxide

H-TeTeTe-SeSe-H
tritellane(diselenoperoxol) (preselected name)
tritelluryl diselenohydroperoxide

C_6H_5-SSS-OH
phenyltrisulfanol (PIN)

CH_3-TeTeTeTe-SH
methyltetratellanethiol (PIN)

P-68.4.1.2 Multiplicative nomenclature is used if conditions for its use are fulfilled. Central substituent groups are derived from the general method for generating divalent substituent groups (see P-29.3.2.2).

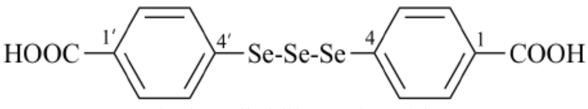
–O-O-O–
trioxidanediyl (preselected prefix)
trioxy

–S-S-S–
trisulfanediyl (preselected prefix)
trithio

–Se-Se-Se-Se–
tetraselanediyl (preselected prefix)
tetraseleno

Examples:

HS-S-S-CH_2-S-S-SH
1,1′-methylenebis(trisulfane) (PIN)



4,4′-triselanediyldibenzoic acid (PIN)
4,4′-triselenodibenzoic acid

P-68.4.1.3 If the chain of identical chalcogen atoms is terminated by one or two acyl groups the compound is named as a pseudoketone (see P-64.1.2.1, P-64.3 and P-65.7.5.1) on the basis of the preferred carbonyl component. Multiplicative nomenclature is used if the principles for its use are met.

Examples:

CH_3-CH_2-CO-O-O-OH
1-trioxidanylpropan-1-one (PIN)
1-hydrotrioxypropan-1-one

CH_3-CH_2-CO-S-S-S-CO-CH_2-CH_3
1,1′-trisulfanediyldi(propan-1-one) (PIN)
1,1′-trithiodi(propan-1-one)

CH_3-CH_2-CO-Se-Se-Se-CH_3
1-(methyltriselanyl)propan-1-one (PIN; a pseudoketone)
(not *Se*-methyldiselanyl propaneselenoate, a pseudoester;
formation of the pseudoester would require the fragmentation of a homogeneous chain)
1-(methyltriseleno)propan-1-one

CH_3-CH_2-CO-S-S-S-S-S-CO-CH_3
1-(acetylpentasulfanyl)propan-1-one (PIN)

P-68.4.2 Three or more heterogeneous contiguous chalcogen atoms

P-68.4.2.1 Compounds of the type a[ba]$_n$ are parent hydrides; they are discussed in P-21.2.3.1.

Examples:

HS-O-SH
dithioxane (preselected name)

CH_3-S-O-SH
methyldithioxane (PIN)
(not methylsulfane-*OS*-thioperoxol)

CH_3-S-O-S-CH_3
dimethyldithioxane (PIN)

C_6H_5-S-O-S-CH_3
methyl(phenyl)dithioxane (PIN)

HS-O-S-OH
dithioxanol (preselected name)
(sulfanyloxy)sulfanol
(not hydroxysulfane-*OS*-thioperoxol)

HO-S-O-S-OH
dithioxanediol (preselected name)
[not oxybis(sulfanol)]

P-68.4.2.2 Compounds of the type R-(chalcogen)$_x$-H where x = 3, 4,..., that cannot be named as alcohols, thiols, ethers, sulfides, hydroperoxides, peroxides, or their chalcogen analogues as described in P-63 are named on the basis of the mononuclear parent hydrides 'oxidane', (H_2O), 'sulfane' (H_2S), etc. and 'dioxidane' (HOOH) , 'disulfane' (HSSH), etc. They are also named using suffixes 'ol' (–OH), 'thiol' (–SH), etc. according to P-63.1.2 and 'peroxol' (–OOH), *SO*-thioperoxol (–SOH), etc. according to P-63.4. A chain of two or three consecutive identical chalcogen atoms must not be broken in the construction of the name. When a choice has to be made, suffixes are chosen in accordance with the seniority order of suffixes, –OH is senior to –OOH (see P-41).

Examples:

HS-OH
sulfanol (preselected name)
(not oxidanethiol)

CH_3-OO-SH
methyldioxidanethiol (PIN)

CH_3-OOO-SH
methyltrioxidanethiol (PIN)

CH_3-O-SOH
methyloxidane-*SO*-thioperoxol (PIN)

CH_3-SS-OH
methyldisulfanol (PIN)

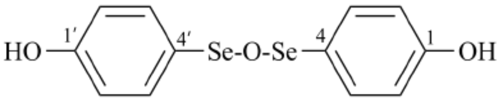
CH_3-SSS-SeH
methyltrisulfaneselenol (PIN)

CH_3-OO-SSH
methyldioxidanedithioperoxol (PIN)

CH_3-O-S-SeSeH
methoxysulfanediselenoperoxol (PIN)

CH_3-SS-OOH
methyldisulfaneperoxol (PIN)

CH_3-S-O-S-OH
[(methylsulfanyl)oxy]sulfanol (PIN)
[not (methylsulfanyl)oxidane-*SO*-thioperoxol]



4,4′-diselenoxanediyldiphenol (PIN)

P-68.4.2.3 Mono-, di- and polynuclear parent hydride names, except for ‘oxidane’ itself, are used for compounds with contiguous chalcogen atoms terminated by hydrogen atoms.

Examples:

HSe-Te-SeH
tellanediselenol (preselected name)
(not selane-*TeSe*-selenotelluroperoxol)

H-OO-S-OH
(hydroperoxy)sulfanol (preselected name)
(not dioxidane-*SO*-peroxol)

H-OO-SS-H
disulfaneperoxol (preselected name)
[(not dioxidane(dithioperoxol)]

P-68.4.2.4 Compounds with an organic group at one or both ends of a heterogeneous chalcogen chain of atoms are named substitutively on the basis of the preferred organic group. Substituting groups may be made up of individual units or formed by functional replacement nomenclature based on tri- or tetraoxy, etc., substituting groups. The latter method is not used if the compound is a pseudoketone. Multiplicative or skeletal replacement (‘a’) nomenclature is used if the requirements for use of either method are met.

Examples:

CH_3-O-S-O-CH_3
[(methoxysulfanyl)oxy]methane (PIN)
(methyl-*OSO*-thiotrioxy)methane
dimethoxysulfane

CH_3-OO-S-CH_3
[(methylperoxy)sulfanyl]methane (PIN)
[not methyl(methylsulfanyl)dioxidane]
(methyl-*OOS*-thiotrioxy)methane

CH_3-S-S-O-CH_2-CH_3
[(methyldisulfanyl)oxy]ethane (PIN)
[methyl(dithioperoxy)oxy]ethane
[not ethoxy(methyl)disulfane]
(methyl-*SSO*-dithiotrioxy)ethane

C_6H_5-O-S-O-C_6H_5
1,1′-[sulfanediylbis(oxy)]dibenzene (PIN)
OSO-thiotrioxydibenzene

CH_3-O-S-Se-C_6H_5
[(methoxysulfanyl)selanyl]benzene (PIN)
methyl-*OSSe*-selenothiotrioxybenzene

$CH_3\text{-S-O-Se-}\overset{1}{C}O\text{-}\overset{2}{C}H_2\text{-}\overset{3}{C}H_3$
1-{[(methylsulfanyl)oxy]selanyl}propan-1-one (PIN)

$\overset{3}{C}H_3\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}O\text{-O-O-S-CO-}CH_3$
1-[(acetylsulfanyl)peroxy]propan-1-one (PIN)

$$\overset{3}{C}H_3\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}O\text{-}O\text{-}S\text{-}S\text{-}O\text{-}\overset{1'}{C}O\text{-}CH_2\text{-}CH_3$$

1,1′-[disulfanediylbis(oxy)]di(propan-1-one) (PIN)
1,1′-[dithioperoxybis(oxy)]di(propan-1-one)

$$\overset{1}{C}H_3\text{-}\overset{2}{C}H_2\text{-}\overset{3}{O}\text{-}\overset{4}{Se}\text{-}\overset{5}{S}\text{-}\overset{6}{O}\text{-}\overset{7}{C}O\text{-}\overset{8}{C}H_2\text{-}\overset{9}{C}H_3$$

3,6-dioxa-5-thia-4-selenanonan-7-one (PIN)

$$\overset{3}{C}H_3\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}Se\text{-}Se\text{-}O\text{-}S\text{-}CH_3$$

1-{[(methylsulfanyl)oxy]selanyl}propane-1-selone (PIN)

$$\overset{3}{C}H_3\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}O\text{-}OO\text{-}S\text{-}CH_3$$

1-[(methylsulfanyl)peroxy]propan-1-one (PIN)

P-68.4.3 Chalcogen parent compounds with nonstandard bonding numbers

Many chalcogen compounds are designated by class names that were used as parent structures to name their derivatives. In these recommendations, in conformity with the principle that substitutive names are preferred, derivatives named on the basis of class names are retained for general use only.

P-68.4.3.1 Sulfanes, selanes, and tellanes
P-68.4.3.2 Di- and polysulfoxides, polysulfones, and selenium and tellurium analogues
P-68.4.3.3 Sulfimides, and chalcogen analogues, $H_2E{=}NH$, where E = S, Se, or Te
P-68.4.3.4 Sulfinylamines, $RN{=}E{=}O$, sulfonylamines, $RN{=}E({=}O)_2$ and chalcogen analogues where E = S, Se, or Te
P-68.4.3.5 Sulfonediimines, $RE({=}NH)_2R'$ and chalcogen compounds where E = S, Se, or Te
P-68.4.3.6 Sulfoximides, $R_2E({=}O){=}NR'$ and chalcogen analogues where E= S, Se, or Te
P-68.4.3.7 Sulfur diimides, $HN{=}E{=}NH$ and chalcogen analogues where E = S, Se, or Te)
P-68.4.3.8 Sulfur triimides, $E({=}NH)_3$ and chalcogen analogues where E= S, Se, or Te)

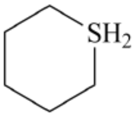
P-68.4.3.1 Sulfanes, selanes, and tellanes

Sulfanes, selanes, and tellanes that have a nonstandard bonding number are named on the basis of parent hydrides such as λ^4-sulfane, λ^6-sulfane, and λ^4-selane, according to the λ-convention.

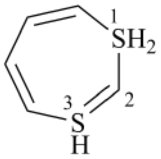
Examples:

$CH_2{=}S(CH_3)_2$
dimethyl(methylidene)-λ^4-sulfane (PIN)

$(CH_3\text{-}O)_4S$
tetramethoxy-λ^4-sulfane (PIN)
[(trimethoxy-λ^4-sulfanyl)oxy]methane



λ^4-thiane (PIN)



1*H*-1λ^4,3λ^4-dithiepine (PIN)

P-68.4.3.2 Di- and polysulfoxides, polysulfones, and selenium and tellurium analogues

Compounds with the general structures $R\text{-}[SO]_n\text{-}R'$ and $R\text{-}[SO_2]_n\text{-}R'$, in which $n \geq 2$, have the class name ‘disulfoxides’, ‘trisulfoxides’, ‘disulfones’, etc. They and their selenium and tellurium analogues are named in two ways:

(1) substitutively by adding the suffix ‘one’ to the name of the appropriate parent hydride, λ^4 or λ^6 disulfane, diselane, ditellane, etc.;

(2) by functional class nomenclature, using class names such as ‘disulfoxide’, ‘disulfone’, ‘diselenoxide’, ‘diselenone’, etc.

Method (1) generates preferred IUPAC names and is also used to name mixed sulfoxide-sulfones.

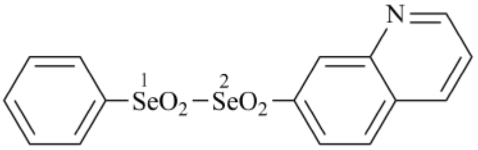
Examples:

$$CH_3\text{-}\overset{1}{S}(=O)\text{-}\overset{2}{S}(=O)\text{-}CH_3$$

1,2-dimethyl-1λ^4,2λ^4-disulfane-1,2-dione (PIN)
dimethyl disulfoxide

$$CH_3\text{-}CH_2\text{-}\overset{1}{S}O_2\text{-}\overset{2}{S}O_2\text{-}CH_3$$

1-ethyl-2-methyl-1λ^6,2λ^6-disulfane-1,1,2,2-tetrone (PIN)
ethyl methyl disulfone



1-phenyl-2-(quinolin-7-yl)-1λ^6,2λ^6-diselane-1,1,2,2-tetrone (PIN)
phenyl quinolin-7-yl diselenone

$$CH_3\text{-}CH_2\text{-}\overset{1}{Se}O_2\text{-}\overset{2}{Se}(O)\text{-}CH_2\text{-}CH_3$$

diethyl-1λ^6,2λ^4-diselane-1,1,2-trione (PIN)
[(ethaneseleninyl)selenonyl]ethane
[(ethylseleninyl)selenonyl]ethane

P-68.4.3.3 Sulfimides and chalcogen analogues, $H_2E{=}NH$, where E = S, Se, or Te

Compounds with the general structures, $H_2S{=}NH$, belong to a class called ‘sulfimides’ (CAS calls them sulfilimines). They are named in two ways:

(1) substitutively by adding the suffix ‘imine’ to the name of the parent hydride such as λ^4-sulfane;

(2) substitutively using the class name ‘sulfimide’.

Method (1) generates preferred IUPAC names.

Example:

$$(C_2H_5)_2\overset{S}{S}{=}\overset{N}{N}\text{-}C_6H_5$$

S,*S*-diethyl-*N*-phenyl-λ^4-sulfanimine (PIN)
S,*S*-diethyl-*N*-phenylsulfimide

N and/or *S* substitution by groups that are not hydrocarbyl groups, may create senior parent structures that become the basis for the name.

Example:

$$(C_6H_5)_2S{=}\overset{N}{N}\text{-}SO_2\text{-}C_6H_5$$

N-(diphenyl-λ^4-sulfanylidene)benzenesulfonamide (PIN)
S,*S*-diphenyl-*N*-(benzenesulfonyl)sulfimide

P-68.4.3.4 Sulfinylamines, RN=E=O, sulfonylamines, RN=E(=O)$_2$ and chalcogen analogues where E = S, Se, Te.

Compounds with the general structures, R-N=S=O and R-N=S(=O)$_2$, have the class names ‘sulfinylamines’ and ‘sulfonylamines’, respectively. They are named substitutively on the basis of the parent hydrides λ^4-sulfane or λ^6-sulfane.

Examples:

$C_6H_5\text{-}N{=}S{=}O$
(phenylimino)-λ^4-sulfanone (PIN)
(not *N*-sulfinylaniline)

$CH_3\text{-}N{=}S(=O)_2$
(methylimino)-λ^6-sulfanedione (PIN)
(not *N*-sulfonylmethanamine)

$(CH_3)_2S(O){=}N\text{-}SO_2\text{-}C_6H_5$
N-[dimethyl(oxo)-λ^6-sulfanylidene]benzenesulfonamide (PIN)
(benzenesulfonylimino)dimethyl-λ^6-sulfanone

P-68.4.3.5 Sulfonediimines, RE(=NH)$_2$R′, and chalcogen analogues where E = S, Se, or Te.

Compounds with the general structures, $RE(=NH)_2R'$, have the class name ‘sulfonediimines’. Preferred IUPAC names are formed substitutively on the basis of the parent hydride λ^6-sulfane. Names based on the class name ‘sulfonediimine’ are not recommended.

Example:

$(C_6H_5)_2S(=NH)_2$
diphenyl-λ^6-sulfanediimine (PIN)
(not diphenyl sulfonediimine)

P-68.4.3.6 Sulfoximides, $R_2E(=O)=NR'$ (E = S), and chalcogen analogues where E = Se, Te.

Compounds with the general structure $R_2E(=O)=NR'$ have the class name ‘sulfoximides’ (CAS calls them sulfoximines). Preferred IUPAC names are formed substitutively on the basis of the parent hydride λ^6-sulfane. Substitutive names may also be based on the functional parent name ‘sulfoximide’.

Example:

$(CH_3)_2S(=O)=N\text{-}C_6H_5$
dimethyl(phenylimino)-λ^6-sulfanone (PIN)
S,*S*-dimethyl-*N*-phenylsulfoximide

P-68.4.3.7 Sulfur dimides, HN=E=NH and chalcogen analogues where E = Se, Te

Compounds with the general structure, HN=S=NH, belong to a general class having the the class name ‘sulfur diimides’. Preferred IUPAC names are formed substitutively on the basis of the parent hydride λ^4-sulfane. Functional class names are based on the class name ‘sulfur diimide’.

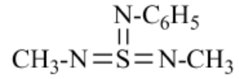
Example:

$CH_3\text{-}N=S=N\text{-}CH_2\text{-}CH_3$
ethyl(methyl)-λ^4-sulfanediimine (PIN)
ethylmethylsulfur diimide

P-68.4.3.8 Sulfur triimides, $E(=NH)_3$, and chalcogen analogues where E = S, Se or Te

Compounds with the general structure, $S(=NH)_3$, belong to a general class called ‘sulfur triimides’. Preferred IUPAC names are formed substitutively on the basis of the parent hydride λ^6-sulfane. Functional class names are based on the class name ‘sulfur triimide’.

Example:



$$CH_3\text{-}N=\overset{\overset{\displaystyle N\text{-}C_6H_5}{\|}}{S}=N\text{-}CH_3$$

dimethyl(phenyl)-λ^6-sulfanetriimine (PIN)
dimethyl(phenyl)sulfur triimide

P-68.5 NOMENCLATURE FOR COMPOUNDS OF THE GROUP 17 ELEMENTS

P-68.5.0 Substitutive nomenclature
P-68.5.1 Nomenclature based on halogen parent hydrides
P-68.5.2 Nomenclature of halogen acids
P-68.5.3 Amides of halogen acids

P-68.5.0 Substitutive nomenclature

In substitutive nomenclature, halogen atoms are denoted only by specific prefixes (see P-61.3), in functional class nomenclature by their class name (see P-15.2), and in functional replacement nomenclature by prefixes and infixes (see P-65.2.1.5).

Examples:

$CH_3\text{-}Cl$
chloromethane (PIN)
methyl chloride

$C_6H_5\text{-}ClO$
chlorosylbenzene (PIN)

$CH_3\text{-}CH_2\text{-}CO\text{-}Br$
propanoyl bromide (PIN)
propionyl bromide

CH_3-CH_2-SO_2-Cl
ethanesulfonyl chloride (PIN)

C_6H_5-P(O)Cl_2
phenylphosphonic dichloride (PIN)

CH_3-BCl_2
dichloro(methyl)borane (PIN)

$CH_3P(Cl)(S$-$C_2H_5)$
ethyl methylphosphonochloridothioite
(not ethyl methanephosphonochloridothioite)

P-68.5.1 Nomenclature based on halogen parent hydrides

For cyclic and acyclic parent hydrides the lambda convention is used to indicate nonstandard bonding numbers.

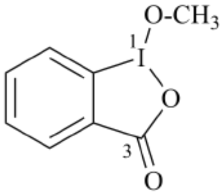
Examples:

C_6H_5-I$(OH)_2$
phenyl-λ^3-iodanediol (PIN)

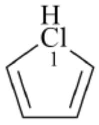
CH_3-ICl_2
dichloro(methyl)-λ^3-iodane (PIN)

$(CH_3$-CO-O$)_2$I–
bis(acetyloxy)-λ^3-iodanyl (preferred prefix)
(not diacetoxyiodo)

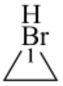
$(HO)_2$I–
dihydroxy-λ^3-iodanyl (preselected name)



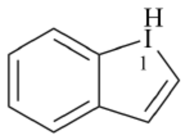
1-methoxy-1λ^3,2-benziodoxol-3(1*H*)-one (PIN)



1*H*-1λ^3-chlorole (PIN)



1λ^3-bromirane (PIN)



1*H*-1λ^3-benziodole (PIN)

P-68.5.2 Nomenclature of halogen acids

The halogen acids HO-Cl, hypochlorous acid, HO-ClO, chlorous acid, HO-ClO_2, chloric acid, and HO-ClO_3, perchloric acid, and similar acids where Br, F, and I take the place of Cl, are discussed in P-67.1.1. They form esters (see P-67.1.3.2), such as 'methyl chlorite', CH_3-O-ClO, and anhydrides (see P-67.1.3.3), such as 'benzoic hypochlorous anhydride', C_6H_5-CO-O-Cl.

Substituent groups derived from the halogen acids, such as chlorosyl, -ClO, bromyl, -BrO_2, and periodyl, -IO_3, are discussed in P-67.1.4.5 and exemplified in P-61.3.2.3.

P-68.5.3 Amides of halogen acids

The seniority order of classes (P-41) is applied to give preferred IUPAC names for amides of halogen acids.

Examples:

CH_3-NH-BrO_2
methylbromic amide (PIN)
N-bromylmethanamine

CH_3-CH_2-NH-Cl
ethylhypochlorous amide (PIN, see P-62.4)
N-chloroethanamine

P-69 NOMENCLATURE FOR ORGANOMETALLIC COMPOUNDS

P-69.0 Introduction
P-69.1 Organometallic compounds involving the elements in Groups 13 through 16
P-69.2 Organometallic compounds involving the elements in Groups 3 through 12
P-69.3 Organometallic compounds involving the elements in Groups 1 and 2
P-69.4 Metallacycles
P-69.5 Seniority order for organometallic compounds

P-69.0 INTRODUCTION

This Section is partly an application of the principles, rules, and conventions established in previous Chapters, and partly an extension of these principles, rules, and conventions to reconcile the nomenclatures of organic and inorganic compounds (see ref. 12) to name organometallic compounds.

Organometallic compounds are compounds having at least one bond between one metal atom and one carbon atom. In addition to the traditional metals, some compounds containing elements such as boron, arsenic, and selenium linked to a carbon atom have sometimes been considered to be organometallic.

Organometallic nomenclature in these recommendations is divided into three categories:

(1) organometallic compounds involving the elements of Groups 1 and 2;

(2) organometallic compounds involving the elements of Groups 3-12 (the transition metals); and

(3) organometallic compounds involving the elements of Groups 13 through 16.

Thus, a great part of nomenclature of organometallic compounds is outside the scope of this book, which deals with organic compounds; it follows the principles, rules and conventions of the nomenclature of inorganic compounds described in the Nomenclature of Inorganic Chemistry (Red Book), in particular, Chapter IR-10 , ref. 12.

All organometallic compounds can be named by a type of additive nomenclature conveniently called coordination nomenclature, a system in which the names of compounds are formed by adding the name(s) of (a) ligand(s), in alphanumerical order if there is more than one, to that of a central atom (ref. 12, Chapters IR-7, IR-9). However, organometallic compounds involving the elements of the Groups 13 through 16 can also be named by using substitutive nomenclature, as shown in Section P-68.

In this Section, all organometallic compounds are considered, first, those involving the elements of Groups 13 through 16 that are named substitutively, then those of the transition elements (Groups 3 through 12) and of Groups 1 and 2, that are named additively. Finally, the seniority rules necessary to name compounds that fall into both caregories are discussed.

Preferred IUPAC names are indicated for organometallic compounds named substitutively for the metals in Groups 14-16. However, neither preferred IUPAC names or preselected names (see P-12.2) for organometallic compounds involving the transition elements (including the Group 3 elements) and Groups 1 and 2 elements, except for ‘ocene’ compounds, are noted. This determination will await consideration by a task group on inorganic and/or organometallic nomenclature.

P-69.1 ORGANOMETALLIC COMPOUNDS INVOLVING THE ELEMENTS OF GROUPS 13 THROUGH 16

Organometallic compounds involving the elements of Groups 13, 14, 15, and 16 are named substitutively by prefixing the appropriate substituent names to the name of a parent hydride. Principles, rules, and conventions to name them have been discussed in Section P-68.

Examples:

$Al(CH_2$-$CH_3)_3$
triethylalumane (substitutive name)

$Pb(CH_2$-$CH_3)_4$
tetraethylplumbane (PIN; substitutive name)

$BrSb(CH{=}CH_2)_2$
bromodi(ethenyl)stibane (PIN; substitutive name)

$HIn(CH_3)_2$
dimethylindigane (substitutive name)

P-69.2 ORGANOMETALLIC COMPOUNDS INVOLVING THE ELEMENTS IN GROUPS 3 THROUGH 12

P-69.2.1 Coordination nomenclature is the primary nomenclature method used to name organometallic compounds containing elements of Groups 3 through 12. It is described in *Nomenclature of Inorganic Chemistry* (IR-10, ref. 12). It is discussed briefly and exemplified in this Section.

P-69.2.2 Definitions of terms

In the rules that follow, certain terms are used in the sense indicated here. A '**coordination entity**' refers to molecules or ions in which there is an atom (A) to which attached other atoms (B) or groups (C). The atom (A) is known as the '**central atom**', and all other atoms which are directly attached to (A) are called '**ligands**'. Each central atom (A) has a '**coordination number**' which is the number of atoms directly attached to it. A group containing more than one potential coordinating atom is termed a '**multidentate**' ligand, the number of potential coordinating atoms being indicated by the terms '**monodentate**', '**bidentate**', etc. A '**chelate**' ligand is a group attached to the central atom through two or more coordinating atoms, while a '**bridging group**' is attached to more than one center of coordination. A '**polynuclear**' coordination entity is one that contains more than one central atom, their number being designated by the terms '**mononuclear**', '**dinuclear**', etc., molecule.

Linear formulae are composed of the symbol of the central atom, followed by the ligands, in alphabetical order (as written) if more than one is present (IR-4.4.3.2, ref. 12). [This is a change from that described in the 1990 Inorganic Nomenclature recommendations.] In a line formula, a coordination entity is always placed in square brackets. No brackets are required when the structure is based on developed organic formulas. Abbreviations are used to represent complicated organic ligands in formulae (although they should not be used in names), for example Et = ethyl, ox = ethanedioato or oxalato, and py = pyridine; (see IR-4.4.3.2 and Tables VII and VIII, ref. 12).

In names of coordination compounds, the name of the central atom is placed after that of the ligand(s), which are listed in alphabetical order, regardless of the number of each. A compound or complex ligand is treated as a single unit. The names of anionic ligands, whether organic or inorganic, end in 'o'. If the anion name ends in 'ate', 'ite', or 'ide', the final letter 'e' is replaced by 'o', giving 'ato', 'ito', or 'ido'.

Examples:

CH_3^-
methanido (for the suffix 'ide', see P-72.2.2.1)

$C_6H_5^-$
benzenido

$(CH_3)_2As^-$
dimethylarsanido

$CH_3\text{-}COO^-$
acetato (for the ending 'ate', see P-65.6.1)

Because of a long established tradition, names for substituent groups as defined in Section P-29 can also be used as ligand names.

Examples:

CH_3^-
methyl

$C_6H_5^-$
phenyl

$(CH_3)_3Si^-$
trimethylsilyl

The name of a coordinated molecule (neutral ligand) or of a cation as a ligand is used without change.

Examples:

$(CH_3\text{-}CH_2)_3P$
triethylphosphane

$CH_3\text{-}NH_2$
methanamine

Exceptionally, the molecules H_2O, NH_3, CO, and NO are named ‘aqua’, ‘ammine’, ‘carbonyl’, and ‘nitrosyl’ when used as ligands.

P-69.2.3 Compounds with at least one metal-carbon single bond

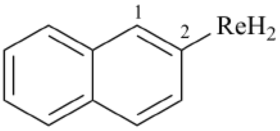
Compounds are named by citing the names of ligands, including hydrogen atom(s), in alphanumerical order, followed by the name of the metal. The presence of hydrogen attached to a metal atom must always be indicated by the prefix ‘hydrido’.

Examples:

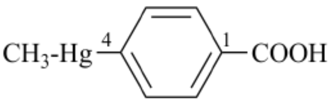
$[Ti(CH_3)Cl_3]$
trichlorido(methanido)titanium
trichlorido(methyl)titanium

$[Pt\{C(O)\text{-}CH_3\}(CH_3)(PEt_3)_2]$
acetyl(methanido)bis(triethylphosphane)platinum
acetyl(methyl)bis(triethylphosphane)platinum

$[Os(CH_2\text{-}CH_3)(NH_3)_5]Cl$
pentaammine(ethanido)osmium(1+) chloride
pentaammine(ethyl)osmium(1+) chloride



dihydrido(naphthalen-2-ido)rhenium
dihydrido(naphthalen-2-yl)rhenium

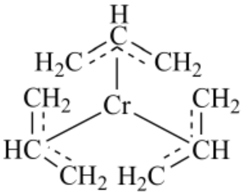


(4-carboxybenzenido)methanidomercury
(4-carboxyphenyl)(methyl)mercury

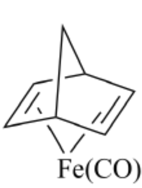
P-69.2.4 Organometallic groups with multicenter bonding to carbon atoms

In order to indicate multicenter bonding to carbon atoms, for example in an unsaturated system, the name of the ligand is preceded by the prefix η (eta). A right superscript is added to the symbol η to indicate the number of atoms that bind to the metal. When it is necessary to indicate that not all unsaturation sites are bonded to the metal, numerical locants are added in front of the symbol η. It may also be necessary to denote a single atom in the ligand that is directly attached to the metal; in this case, the symbol κ (kappa) is cited before the element symbol that indicates the specific position that is bonded to the metal. See IR-10.2.5.1 and IR-10.2.3.3 (ref. 12) for a complete discussion on the use of η and κ symbols in additive nomenclature.

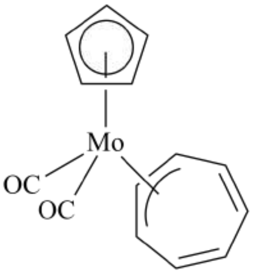
Examples:



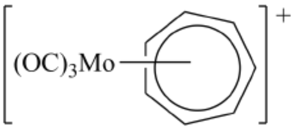
tris(η^3-allyl)chromium



[(2,3,5,6-η)-bicyclo[2.2.1]hepta-2,5-diene]tricarbonyliron



dicarbonyl[(1−3-η)-cyclohepta-2,4,6-trien-1-ido](η^5-cyclopenta-2,4-dien-1-ido)molybdenum
dicarbonyl[(1−3-η)-cyclohepta-2,4,6-trien-1-yl](η^5-cyclopenta-2,4-dien-1-yl)molybdenum
dicarbonyl[(1−3-η)-cyclohepta-2,4,6-trien-1-ido](η^5-cyclopentadienido)molybdenum

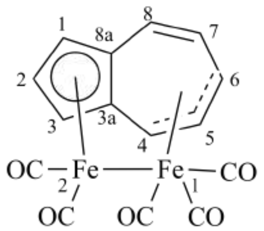


tricarbonyl(η^7-cycloheptatrienylium)molybdenum(1+)
tricarbonyl(η^7-cyclohepta-2,4,6-trien-1-ylium)molybdenum(1+)

P-69.2.5 Bridging organometallic groups with multicenter bonding to carbon atoms

The prefix ‘μ’ (see IR-9.2.5.2, ref. 12) is added at the front of the name of a bridging ligand to indicate bridging between two metal atoms. Locants for the ‘η’ positions are separated by a colon and a hyphen is added following the name of the bridging group. Direct bonding between metal atoms is indicated as described in IR-10.2.5.1 (ref. 12).

Example:

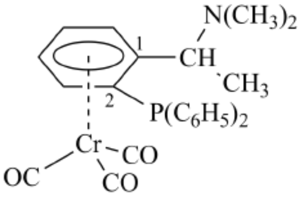


{μ-[2(1–3,3a,8a-η):1(4−6-η)]azulene}-(pentacarbonyl-1| ^{3}*C*,2| ^{2}*C*)diiron(*Fe*—*Fe*)

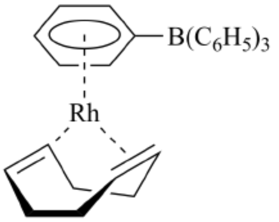
P-69.2.6 Organometallic compounds with unsaturated molecules and substituent groups

Organic molecules used as ligands are named substitutively in accordance with principles, rules. and conventions of substitutive nomenclature and cited in the name of the organometallic compound with the appropriate ‘η’ (hapto) symbols. This method is preferred to that consisting of using prefixes only to denote characteristic groups in the organic part of the organometallic compound.

Examples:



tricarbonyl{1-[2-(diphenylphosphanyl)-η^6-phenyl]-*N*,*N*-dimethylethan-1-amine}chromium

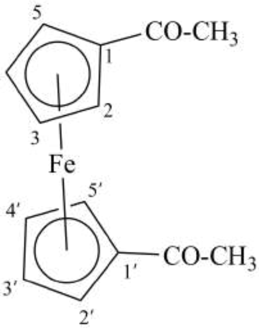


[(1,2,5,6-η)-cycloocta-1,5-diene][triphenyl(η^6-phenyl)boranuido]rhodium
[(1,2,5,6-η)-cycloocta-1,5-diene][triphenyl(η^6-phenyl)borato]rhodium

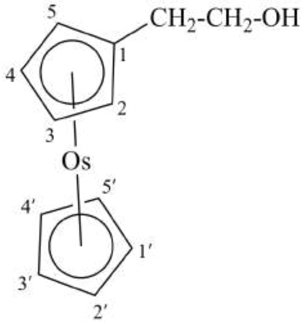
P-69.2.7 “Ocenes”

“Ocenes” are bis(η^5-cyclopenta-2,4-dien-1-ido) or bis(η^5-cyclopenta-2,4-dien-1-yl) or bis(η^5-cyclopentadienido) complexes of certain metals. The names ferrocene, ruthenocene, osmocene, nickelocene, chromocene, cobaltocene, and vanadocene are names for compounds corresponding to ‘bis(λ^5-cyclopenta-2,4-dien-1-yl)metal’, where the metal atom is Fe, Ru, Os, Ni, Cr, Co, and V. Ocenes are considered as heterocycles and seniority is based on the extension of the list of seniority for heterocycles through Groups 12, 11, 10, 9, 8, 7, 6, 5, 4, 3, 2, 1, for example nickelocene > cobaltocene > ferrocene. These names are substituted in accordance with the principles, rules, and conventions of substitutive nomenclature, using suffixes or prefixes to denote characteristic groups.

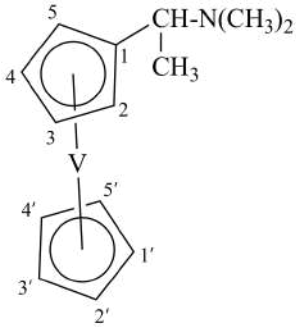
Examples:


CO-CH3
Fe
CO-CH3

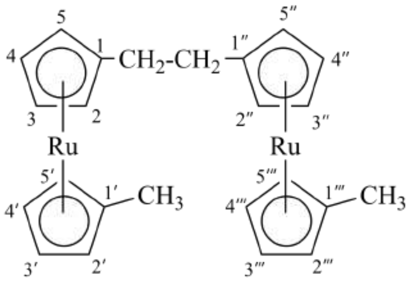
1,1′-(ferrocene-1,1′-diyl)di(ethan-1-one) (PIN)
1,1′-diacetylferrocene


CH2-CH2-OH
Os

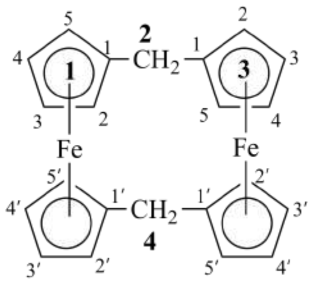
2-(osmocen-1-yl)ethanol (PIN)
1-(2-hydroxyethyl)osmocene


CH-N(CH3)2
CH3
V

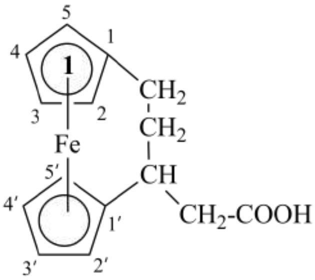
N,*N*-dimethyl-1-vanadocenylethan-1-amine (PIN)
[1-(dimethylamino)ethyl]vanadocene


CH2-CH2
Ru
Ru
CH3
CH3

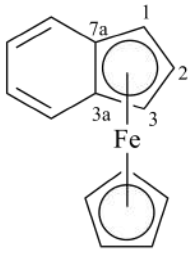
1,1″-(ethane-1,2-diyl)bis(1′-methylruthenocene) (PIN)


1
2
3
4
CH2
CH2
Fe
Fe

1,3(1,1′)-diferrocenacyclotetraphane (PIN)



3,5-(ferrocene-1,1′-diyl)pentanoic acid (PIN)
1,1′-(4-carboxybutane-1,3-diyl)ferrocene



benzoferrocene (PIN)
(η^5-cyclopenta-2,4-dien-1-ido)[(1,2,3,3a,7a)-η^5-1*H*-inden-1-ido]iron
(η^5-cyclopenta-2,4-dien-1-yl)[(1,2,3,3a,7a)-η^5-1*H*-inden-1-yl]iron
(η^5-cyclopentadienido)[(1,2,3,3a,7a)-η^5-indenido]iron

P-69.3 ORGANOMETALLIC COMPOUNDS INVOLVING THE ELEMENTS IN GROUPS 1 AND 2

Although many organometallic compounds of Groups 1 and 2 elements exist in associated molecular form and contain structural solvent, their names are based on the stoichiometric compositions of the compounds, the solvent, if any, being ignored. Additive names are formed by citing the names of the ligands denoting the organic groups and the ligand ‘hydrido’ denoting the hydrogen atoms, if any, in alphabetical order, followed by the name of the metal.

Examples:

[BeEtH]
ethylhydridoberyllium
ethanidohydridoberyllium

$NaCH=CH_2$ or$[Na(CH=CH_2)]$
ethenidosodium
ethenylsodium
vinylsodium
(sodium ethenide is also acceptable;
it is a compositional name analogous to sodium chloride; see IR-5, ref. 12)

[LiMe]
methanidolithium
methyllithium

$[(LiMe)_4]$
tetra-μ_3-methanido-tetralithium
tetra-μ_3-methyl-tetralithium

$(LiMe)_n$
poly(methyllithium)
poly(methanidolithium)

LiMe
lithium methanide (compositional name; see IR-5, ref. 12)

[MgI(Me)]
iodido(methanido)magnesium
(additive name of coordination type)

[MgMe]I
methylmagnesium iodide (compositional name;
the formally electropositive component named by additive nomenclature)

$[MgI(Me)]_n$
poly[iodido(methanido)magnesium], or
poly[iodido(methyl)magnesium]

MgIMe
magnesium iodide methanide
(compositional name, see IR-5, ref. 12)

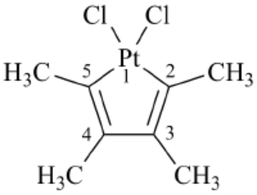
P-69.4 METALLACYCLES

Metallacycles are organic heterocycles in which one or more heteroatoms is (are) metal atoms other than the metals normally included in the nomenclature systems for heteromonocycles (see P-22.2). They may be named by extending the Hantzsch-Widman system to include the metallic elements in addition to those in Groups 13 through 16, but with a '0' standard valence and the stems described in Table 2.5, for example 'ine' and 'inane' for unsaturated and saturated six-membered heterocycles, respectively or by selecting a parent hydrocarbon ring or ring system and replacing one or more carbon atoms by a metal atom from Groups 2 through 12 using a nondetachable skeletal replacement ('a') prefix to create the metallacyclic parent hydride. The name is adjusted to conform to the observed formula by substitutions using detachable prefixes on the ring and appropriate ligand names to describe atoms or groups attached to the metal atom.

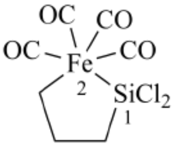
The option to include the metallic elements in addition to the metals in Groups 13 through 16 in the Hantzsch-Widman system and their skeletal replacement ('a') prefixes is a major change from previous recommendations on the Hantzsch-Widman system.

Note: A project to consider the nomenclature for metallacycles containing transition metals has been established.

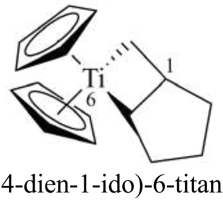
Examples:



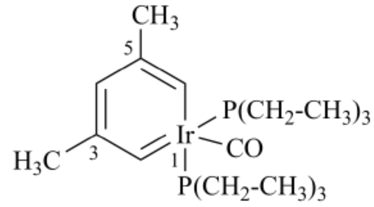
1,1-dichloro-2,3,4,5-tetramethylplatinole
(Hantzsch-Widman type name)
1,1-dichloro-2,3,4,5-tetramethyl-1-platinacyclopenta-2,4-diene
(skeletal replacement name)



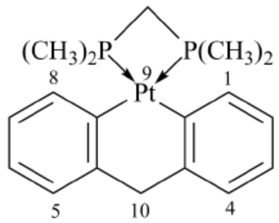
2,2,2,2-tetracarbonyl-1,1-dichloro-1,2-silaferrolane
(Hantzsch-Widman type name)
2,2,2,2-tetracarbonyl-1,1-dichloro-1-sila-2-ferracyclopentane
(skeletal replacement name)



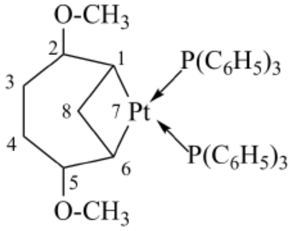
6,6-di(η^5-cyclopenta-2,4-dien-1-ido)-6-titanabicyclo[3.2.0]heptane
(skeletal replacement name)
6,6-di(η^5-cyclopentadienyl)-6-titanabicyclo[3.2.0]heptane
(skeletal replacement name)
6,6-di(η^5-cyclopentadienido)-6-titanabicyclo[3.2.0]heptane
(skeletal replacement name)



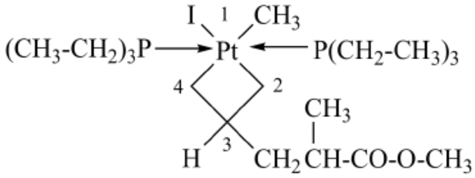
1-carbonyl-3,5-dimethyl-1,1-bis(triethylphosphane)-1-iridabenzene
(skeletal replacement name)



9,9-[methylenebis(dimethylphosphane)]-10*H*-9-platinaanthracene
(skeletal replacement name)



2,5-dimethoxy-7,7-bis(triphenylphosphane)-7-platinabicyclo[4.1.1]octane
(skeletal replacement name)



methyl 3-[1-iodo-1-methyl-1,1-bis(triethylphosphane)platinetan-3-yl]-2-methylpropanoate
(Hantzsch-Widman name)
methyl 3-[1-iodido-1-methanido-1,1-bis(triethylphosphane)platinetan-3-yl]-2-methylpropanoate
(Hantzsch-Widman name)
methyl 3-[1-iodo-1-methyl-1,1-bis(triethylphosphane)-1-platinacyclobutan-3-yl]-2-methylpropanoate
(skeletal replacement name)

P-69.5 SENIORITY ORDER FOR ORGANOMETALLIC COMPOUNDS

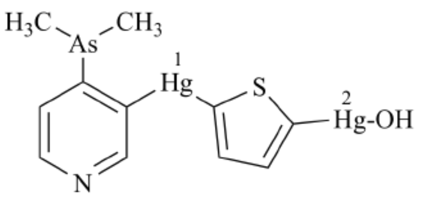
When two different metals are present in an organometallic compound, one must be chosen as the basis of the name. Metals are classified into:

(1) metals of Groups 1 through 12; and

(2) metals of Groups 13 through 16.

P-69.5.1 Compounds having two identical or different metal atoms belonging to the first class are named additively using the methodology described in Section IR-9.2.5 of ref. 12, and the order of seniority of the Element Sequence Table beginning at Zn, i.e. Zn > Cd > Hg >.....Li > Na > K > Rb > Cs > Fr (see Table VI, ref. 12).

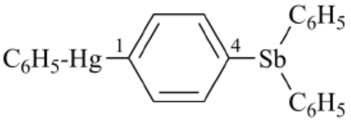
Example:



1-[4-(dimethylarsanyl)pyridin-3-yl]-2-hydroxido-μ-thiophene-2,5-diyl-dimercury

P-69.5.2 Compounds having one metal atom of class (1) and another atom of class (2) are named additively using the metal atom of class (1) as central atom, as in P-69.5.1; the other metal atom is named as a substituent group in substitutive nomenclature or as a neutral ligand.

Example:



[4-(diphenylstibanyl)phenyl](phenyl)mercury

P-69.5.3 For organometallic compounds having two metal atoms belonging to class (2), substitutive nomenclature is used, as described in Section P-68. The order of priority to select the parent hydride is described in Section P-41: Sb > Bi > Ge > Sn > Pb > Al > Ga > In > Tl.

Examples:

$(C_6H_5)_2Bi\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}Pb(C_2H_5)_3$
diphenyl[3-(triethylplumbyl)propyl]bismuthane (PIN)

$H_2Bi\text{-}GeH_3$
germylbismuthane

$Pb(SnH_3)_4$
plumbanetetrayltetrakis(stannane)

International Union of Pure and Applied Chemistry

Division VIII Chemical Nomenclature and Structure Representation Division

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Chapter P-7 RADICALS, IONS, AND RELATED SPECIES

P-70 Introduction
P-71 Radicals
P-72 Anions
P-73 Cations
P-74 Zwitterions
P-75 Radical ions
P-76 Delocalized radicals and ions
P-77 Salts

P-70 INTRODUCTION

P-70.1 General Methodology
P-70.2 Seniority of radicals and ions
P-70.3 Name formation
P-70.4 General rules for the selection of preferred names

P-70.1 GENERAL METHODOLOGY.

The nomenclature for radicals, ions and related species is described in this Chapter. Its rules are based on the same principles as those of organic compounds defined in the Chapters P-1 to P-6. The nomenclature was revised in 1993 (ref. 3). For definitions, symbols and conventions, see ref. 14; see also ref. 28. In the 1979 recommendations (ref. 1), radicals were called ‘free radicals’ to distinguish them from substituent prefixes which were also called radicals. That distinction was dropped in the 1993 publications (refs. 2, 3).

P-70.2 SENIORITY OF RADICALS AND IONS

As classes, radicals and ions are senior to acids and other classes in the following order:

(1) radicals;
(2) anions;
(3) cations.

P-70.3 NAME FORMATION

Substitutive names and functional class names denote radicals and ions and related compounds. Parent hydrides and parent compounds are selected and modified by use of specific suffixes (called cumulative suffixes) and prefixes; traditional endings are used to describe anions derived from acids and related compounds (see P-72.2.2.2). The nomenclature of di- and trivalent radicals does not indicate nor imply an electronic structure or spin multiplicity.

P-70.3.1 Suffixes, prefixes, and endings for radicals and ions in substitutive nomenclature are listed in Table 7.1. They are also described in Table 3.4.

Table 7.1 Suffixes or Endings and Prefixes for Radicals and Ions in Substitutive Nomenclature

Operation	Suffix or Ending	Prefix
Radicals formed by		
loss of H•	yl	ylo
loss of 2 H•		
from one atom	ylidene	
from different atoms	diyl	
loss of 3 H•		
from one atom	ylidyne	
from different atoms	triyl or ylylidene	
addition of H•	hydryl	
Anions formed by		

loss of H^+	ide
	ate, ite (endings)
addition of H^-	uide
addition of an electron	elide [1]
Cations formed by	
loss of H^-	ylium
addition of H^+	ium
loss of an electron	elium [1]

[1] The suffixes ‘elide’ and ‘elium’ are recommended to denote modification of a parent hydride by the addition or the subtraction of one electron, respectively.

P-70.3.2 Basic multiplying prefixes are used to denote multiplicity of the suffixes ‘yl’, ‘ylidene’, ‘ylidyne’, ‘ide’, ‘uide’, ‘ium’ and the prefix ‘ylo’. Multiplying prefixes ‘bis’, ‘tris’, etc., are used before the suffix ‘ylium’ and before compound suffixes, such as ‘aminium’, ‘olate’, etc.

P-70.3.3 In names, suffixes and endings are cited in a specific order as described below.

P-70.3.3.1 When two or more cumulative suffixes are present in a name, the order of citation is the reverse of the order of seniority for radicals and ions as given in P-70.2, i.e.,‘ium’, ‘ylium’, ‘ide’, ‘uide’, ‘yl’, ‘ylidene’, ‘ylidyne’.

Example:

$$\mathrm{CH_3\text{-}\underset{3}{N}{=}\underset{\bullet}{\overset{+}{N}}\text{-}\underset{1}{\overset{-}{N}}\text{-}Si(CH_3)_3}$$

3-methyl-1-(trimethylsilyl)triaz-2-en-2-ium-1-id-2-yl (PIN)

P-70.3.3.2 When functional and cumulative suffixes are present, the order of citation is prescribed by specific rules.

P-70.3.3.2.1 A cumulative suffix may be added to a functional suffix to form a defined compound suffix (see P-71.3.2).

Examples:

$$\mathrm{CH_3\text{-}\overset{\bullet}{N}H}$$

methanaminyl (PIN)
methylazanyl
(traditional name: methylamino)

$$\mathrm{\overset{3}{C}H_3\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}H{=}N^{\bullet}}$$

propan-1-iminyl (PIN)
propylideneazanyl

P-70.3.3.2.2 In zwitterionic compounds, cumulative suffixes precede functional suffixes and have seniority for lowest locants:

Example:

$$\mathrm{(CH_3)_3\underset{1}{\overset{+}{N}}\text{-}\underset{2}{N}H\text{-}SO_2\text{-}O^-}$$

1,1,1-trimethylhydrazin-1-ium-2-sulfonate (PIN)

P-70.4 GENERAL RULES FOR THE SELECTION OF PREFERRED NAMES

The concept of preferred IUPAC names as applied to radicals and ions is based on the following principles.

(1) substitutive nomenclature based on carbane and heterane nomenclatures and a set of suffixes and prefixes designed to express the formal operations needed to generate radicals and ions systematically are used to generate preferred IUPAC names; accordingly, the preferred IUPAC name for a radical may not be the same as the preferred prefix.

(2) some names are retained as preferred IUPAC names, notably contracted names such as methoxide, ethoxide, etc., and methoxyl, ethoxyl, etc. related to the substitutive prefixes derived from alcohols and related hydroxy compounds.

(3) some names are retained only for use in general nomenclature, for example the ‘onium cations’ such as ammonium and sulfonium, carbene, $CH_2^{2\bullet}$; amide, NH_2^-; and $CH_3\text{-}C(O)^-$, acetyl anion.

(4) functional class names using class names such as cation, anion, etc. can be used in general nomenclature, but systematically constructed names or retained names are preferred IUPAC names, for example, ‘methylium’ not

‘methyl cation’, for CH_3^+; ‘acetylium’ not ‘acetyl cation’ for CH_3-C(O)$^+$; ‘ethanide’ not ‘ethyl anion’ for CH_3-CH_2; and ‘methaniumyl’ not ‘methyl radical cation’, for $CH_4^{\bullet+}$.

P-71 RADICALS

P-71.1 General methodology
P-71.2 Radicals derived from parent hydrides
P-71.3 Radical centers on characteristic groups
P-71.4 Assemblies of parent radicals
P-71.5 Prefixes denoting radicals
P-71.6 Order of citation and seniority of suffixes ‘yl’, ‘ylidene’, and ‘ylidyne’
P-71.7 Choice of parent radical

P-71.1 GENERAL METHODOLOGY

Radicals are named by modifying a parent hydride name to signal the subtraction or addition of one or more hydrogen atoms, H•. The modification to signal the addition of a single hydrogen atom is recommended for the first time. These two operations are expressed by suffixes.

The suffixes ‘yl’ (–H•), ‘ylidene’ (–2H•), ‘ylidyne’ (–3H•) denote the removal of hydrogen atoms, a subtractive operation.

The suffix ‘hydryl’ denotes the additive operation, i.e., the addition of a single hydrogen atom.

The prefix ‘ylo’ is used to indicate the removal of ‘H•’ from a substituent group, a subtractive operation.

P-71.2 RADICALS DERIVED FROM PARENT HYDRIDES

P-71.2.1 Monovalent radicals.

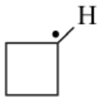
P-71.2.1.1 A radical formally derived by the removal of one hydrogen atom from a mononuclear parent hydride of an element of Group 14, from a terminal atom of an unbranched acyclic hydrocarbon, or from any position of a monocyclic saturated hydrocarbon ring is named by replacing the ‘ane’ ending of the systematic name of the parent hydride by ‘yl’.

Examples:

•CH_3
methyl (PIN)

•CH_2-CH_2-CH_3
propyl (PIN)

•GeH_3
germyl (preselected name)



cyclobutyl (PIN)

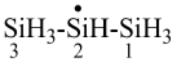
P-71.2.1.2 A radical formally derived by the removal of one hydrogen atom from any position of a parent hydride, or a modified parent hydride other than those described by P-71.2.1.1, above, is named by adding the suffix ‘yl’ to the name of the parent hydride, eliding the final letter ‘e’ of the name of the parent hydride, if any. As an exception, the IUPAC preferred name for HO• is ‘hydroxyl’, a retained name for the systematic name ‘oxidanyl’ (see ref. 12, IR-6.4.7); and the IUPAC preferred name for HOO• is ‘hydroperoxyl’, a retained name for the systematic name ‘dioxidanyl’. These retained names must not be used when substituted, for example, CH_3-O• is named ‘methoxyl’ or ‘methyloxidanyl’, and not ‘methylhydroxyl’ (see P-71.3.4).

Examples:

HS•
sulfanyl (preselected name)

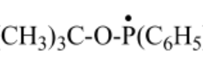
H_2N•
azanyl (preselected name)
aminyl (traditional name: amino)

H_2B•
boranyl (preselected name)
(not boryl)



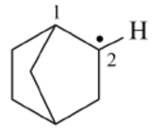
$\underset{3}{\mathrm{SiH_3}}\text{-}\underset{2}{\overset{\bullet}{\mathrm{Si}}\mathrm{H}}\text{-}\underset{1}{\mathrm{SiH_3}}$

trisilan-2-yl (preselected name)

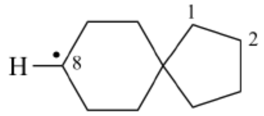


$\mathrm{(CH_3)_3C\text{-}O\text{-}\overset{\bullet}{P}(C_6H_5)_3}$

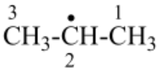
tert-butoxytri(phenyl)-λ^5-phosphanyl (PIN)
[(2-methylpropan-2-yl)oxy]tri(phenyl)-λ^5-phosphanyl
(1,1-dimethylethoxy)tri(phenyl)-λ^5-phosphanyl



bicyclo[2.2.1]heptan-2-yl (PIN)

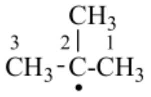


spiro[4.5]decan-8-yl (PIN)



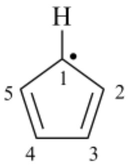
$\overset{3}{\mathrm{CH_3}}\text{-}\underset{2}{\overset{\bullet}{\mathrm{C}}}\mathrm{H}\text{-}\overset{1}{\mathrm{CH_3}}$

propan-2-yl (PIN)
1-methylethyl
isopropyl

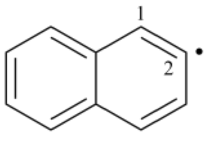


$\overset{3}{\mathrm{CH_3}}\text{-}\underset{\bullet}{\overset{\mathrm{CH_3}}{\overset{2\,|}{\mathrm{C}}}}\text{-}\overset{1}{\mathrm{CH_3}}$

2-methylpropan-2-yl (PIN)
1,1-dimethylethyl
tert-butyl [see P-70.4 (1)]



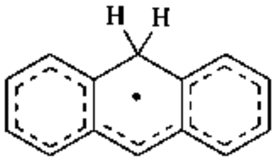
cyclopenta-2,4-dien-1-yl (PIN)
cyclopentadienyl (see P-76)



naphthalen-2-yl (PIN)

P-71.2.1.3 A radical created by the addition of a single hydrogen atom, H•, may be indicated by suffix ‘hydryl’ when the position of the hydrogen atom must be specified:

Example:



anthracene-9-hydryl (PIN)
anthracen-9-iumelide (see P-70.3.1)
anthracen-9-eliumuide (see P-70.3.1)
2,9-dihydroanthracen-2-yl

P-71.2.2 Divalent and trivalent radicals.

The names of divalent and trivalent radicals are formed substitutively using the suffixes ‘ylidene’ and ‘ylidyne’ in two ways:

(1) replacing the ending ‘ane’ of a mononuclear parent hydride of an element of Group 14, or from a terminal atom of an unbranched acyclic hydrocarbon, or from any position of a monocyclic saturated hydrocarbon ring by the appropriate suffix (corresponds to P-71.2.1.1)

(2) adding the appropriate suffix to the name of a parent hydride, other than those described by P-71.2.1.1, at any position eliding the final letter ‘e’ of the name of the parent hydride, if any (corresponds to P-71.2.1.2).

These systematic names are preferred to retained names which may be used in general nomenclature.

P-71.2.2.1 Specific method and retained names

A radical formally derived by the removal of two hydrogen atom from one skeletal atom of a mononuclear parent hydride of an element of Group 14, or from one terminal skeletal atom of an unbranched acyclic hydrocarbon, or from one skeletal atom of a monocyclic saturated hydrocarbon ring is named by replacing the ‘ane’ ending of the systematic name of the parent hydride by the suffix ‘-ylidene’ or ‘-diyl’. The suffix ‘-ylidyne’ or ‘-triyl’ is used to name radicals formally derived by the removal of three hydrogen atoms from a mononuclear parent hydride of an element of Group 14 or from a terminal atom of an unbranched acyclic hydrocarbon.

Systematic names are the preferred IUPAC names. The retained names carbene or methylene, nitrene or aminylene and carbyne, can be used in general nomenclature, with full substitution. The use of the systematic or retained names does not imply a specific electronic configuration. If needed, such a distinction would be made by using a separate word such as singlet or triplet, or a descriptive phrase. The disposition of the two unpaired electrons in the structures is equivalent to that given in the Red Book as $CH_2^{2\bullet}$ (see ref. 12, IR-6.4.7).

Examples:

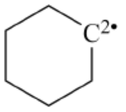
$H_2C^{2\bullet}$
methylidene (PIN)
carbene
methylene

$H_2Si^{2\bullet}$
silylidene (preselected name)
silanediyl
(not silylene)

$HC^{3\bullet}$
methylidyne (PIN)
methanetriyl
carbyne

$(C_6H_5)_2C^{2\bullet}$
diphenylmethylidene (PIN)
diphenylmethanediyl
diphenylcarbene
diphenylmethylene

$C_6H_5\text{-}CH_2\text{-}SiH^{2\bullet}$
benzylsilylidene (PIN)
benzylsilanediyl



cyclohexylidene (PIN)
cyclohexane-1,1-diyl

$CH_3C^{3\bullet}$
ethylidyne (PIN)
ethane-1,1,1-triyl
(not methylcarbyne)

P-71.2.2.2 General method

With the exception of the radicals named in P-71.2.2.1, the names of divalent and trivalent radicals derived by the removal of two or three hydrogen atoms from one position of a parent hydride are formed by adding the suffixes ‘-ylidene’ or ‘-diyl’ and ‘-ylidyne’ or ‘-triyl’, respectively, to the name of the parent hydride, with elision of the final letter ‘e’, if present. The name azanylidene is the preselected name for $HN^{2\bullet}$; nitrene or aminylidene are retained names for use in general nomenclature.

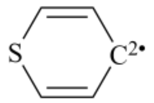
Examples:

$\mathrm{HN}^{2\bullet}$
azanylidene (preselected name)
azanediyl
aminylidene
aminylene
nitrene

$\mathrm{H_2P}^{3\bullet}$
λ^5-phosphanylidyne (preselected name)
λ^5-phosphanetriyl
phosphoranylidyne
phosphoranetriyl

$\mathrm{H_2N\text{-}N}^{2\bullet}$
hydrazinylidene (preselected name)
diazanylidene
hydrazine-1,1-diyl
diazane-1,1-diyl
(traditional name: hydrazono)
(not aminonitrene)

$\mathrm{H_2P\text{-}P}^{2\bullet}$
diphosphanylidene (preselected name)
diphosphane-1,1-diyl

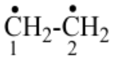


4*H*-thiopyran-4-ylidene (PIN)
4*H*-thiopyran-4,4-diyl

P-71.2.3 Multiple radical centers (polyradicals)

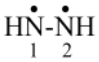
Polyradicals containing two or more radicals centers, formally derived by the removal of two or more hydrogen atoms from each of two or more different skeletal atoms of a parent hydride, are named by adding to the name of the parent hydride combinations of the suffix ‘yl’ for a monovalent radical center, ‘ylidene’ for a divalent radical center, and ‘ylidyne’ for a trivalent radical center, together with the appropriate numerical prefixes indicating the number of each kind of radical center. The final letter ‘e’ of the name of the parent hydride, if present, is elided when followed by ‘y’. All substituents, including characteristic groups, when present, are cited as prefixes. Preferred IUPAC names result from the application of this rule.

Examples:



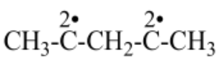
$\underset{1}{\overset{\bullet}{\mathrm{C}}}\mathrm{H_2}\text{-}\underset{2}{\overset{\bullet}{\mathrm{C}}}\mathrm{H_2}$

ethane-1,2-diyl (PIN)
(traditional name: ethylene)



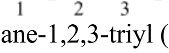
$\mathrm{H}\underset{1}{\overset{\bullet}{\mathrm{N}}}\text{-}\underset{2}{\overset{\bullet}{\mathrm{N}}}\mathrm{H}$

hydrazine-1,2-diyl (preselected name)
diazane-1,2-diyl



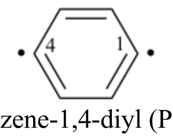
$\mathrm{CH_3}\text{-}\overset{2\bullet}{\mathrm{C}}\text{-}\mathrm{CH_2}\text{-}\overset{2\bullet}{\mathrm{C}}\text{-}\mathrm{CH_3}$

pentane-2,4-diylidene (PIN)

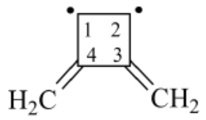


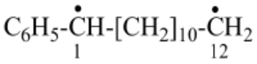
$\underset{1}{\overset{\bullet}{\mathrm{C}}}\mathrm{H_2}\text{-}\underset{2}{\overset{\bullet}{\mathrm{C}}}\mathrm{H}\text{-}\underset{3}{\overset{\bullet}{\mathrm{C}}}\mathrm{H_2}$

propane-1,2,3-triyl (PIN)



benzene-1,4-diyl (PIN)
{traditional names: *p*-phenylene;
1,4-phenylene [see P-70.4 (1)]}


3,4-dimethylidenecyclobutane-1,2-diyl (PIN)


$C_6H_5\text{-}\underset{1}{\overset{\bullet}{C}}H\text{-}[CH_2]_{10}\text{-}\underset{12}{\overset{\bullet}{C}}H_2$

1-phenyldodecane-1,12-diyl (PIN)

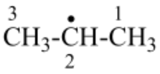
P-71.2.4 Acyclic radicals derived by the removal of one or more hydrogen atoms from nonterminal chain positions are named in two ways:

(1) by citing the locant of the nonterminal position of the chain

(2) by substituting a parent radical that has the free valence(s) at the end of a chain.

Method (1) generates preferred IUPAC names. The principal chain is chosen, if necessary, by the method indicated in Section P-46 for substituent groups.

Example:


$\overset{3}{C}H_3\text{-}\underset{2}{\overset{\bullet}{C}}H\text{-}\overset{1}{C}H_3$

propan-2-yl (PIN)
1-methylethyl

P-71.2.5 The λ-convention

Divalent and trivalent radical centers in a parent hydride formally derived by the removal of two or three hydrogen atoms from the same skeletal atom in its standard valence state may be described by the λ-convention (see P-14.1). Locants for the radical centers are followed by the symbol λ^n, where 'n' is the bonding number of the skeletal atom (see P-14.1). This method is only for general nomenclature.

Examples:

$Cl_2C^{2\bullet}$
dichloro-λ^2-methane
dichloromethylidene (PIN)
dichloromethanediyl

$FC^{3\bullet}$
fluoro-λ^1-methane
fluoromethylidyne (PIN)
fluoromethanetriyl

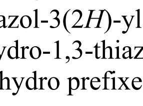
$C_6H_5\text{-}N^{2\bullet}$
phenyl-λ^1-azane
benzenaminylidene (PIN)
phenylazanediyl

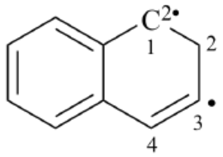
P-71.2.6 'Added indicated hydrogen' for radicals of mancude ring systems

A radical center at a position in a mancude parent hydride where there is an insufficient number of hydrogen atoms to apply directly the recommendations for the use of 'yl' or 'ylidene' given in P-71.2.1 and P-71.2.2 is derived formally from a dihydro derivative of the cyclic parent hydride. Such a radical can also be described by applying the principle of 'added indicated hydrogen' (see P-14.7 and P-58.2). In this method the 'hydro' derivative is described by specifying the hydrogen atom of a dihydro pair that remains after the radical center is created, by citing in italic capital *H* and the locant of the skeletal atom to which the hydrogen atom resides, both enclosed in a set of parentheses and inserted into the name of the corresponding parent hydride immediately after the locant for the radical center.

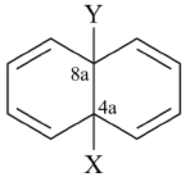
Names formed by the 'added indicated hydrogen' method are preferred to names using 'hydro' prefixes (see P-58.2.5).

Examples:

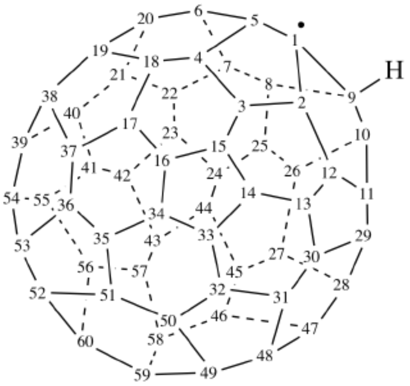

1,3-thiazol-3(2*H*)-yl (PIN)
2,3-dihydro-1,3-thiazol-3-yl
(nondetachable hydro prefixes, see P-58.2.5)



naphthalen-3-yl-1(2*H*)-ylidene (PIN)
1,2-dihydronaphthalen-3-yl-1-ylidene
(nondetachable hydro prefixes; see P-58.2.5)



X = •; Y = H
naphthalen-4a(8a*H*)-yl (PIN)
4a,8a-dihydronaphthalen-4a-yl
(nondetachable hydro prefixes, see P-58.2.5)
X = •; Y = •
naphthalene-4a,8a-diyl (PIN)
4a,8a-dihydronaphthalene-4a,8a-diyl
(nondetachable hydro prefixes, see P-58.2.5)



(C_{60}-I_h)[5,6]fulleren-1(9*H*)-yl (PIN)
1,9-dihydro(C_{60}-I_h)[5,6]fulleren-1-yl
(nondetachable hydro prefixes, see P-58.2.5)

P-71.3 RADICAL CENTERS ON CHARACTERISTIC GROUPS

P-71.3.1 Acyl radicals

Acyl radicals, i.e., radicals with at least one chalcogen or nitrogen atom attached to a radical center by a (formal) double bond, which may be considered to be formally derived by the removal of a hydroxy group from acid characteristic groups, are named by replacing the ‘ic acid’ or ‘carboxylic acid’ ending of the name of the acid with ‘oyl’ or ‘yl’, or ‘carbonyl’, according to the method for forming names of acyl groups (see P-65.1.7). Substituent groups denoted by prefixes such as ‘oxo’, ‘thioxo’, ‘sulfanylidene’, etc., may be used in general nomenclature.

> Compound acyl radicals formed from acyclic parent hydrocarbons and substituent prefixes such as ‘oxo’, ‘thioxo’, ‘sulfanylidene’, and ‘imino’ can be used in general nomenclature; they are used in CAS index nomenclature.

Examples:

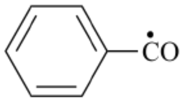
$CH_3\text{-}[CH_2]_4\text{-}\dot{C}O$
hexanoyl (PIN)
1-oxohexyl

$(CH_3)_2\dot{P}O$
dimethylphosphinoyl (PIN)
dimethyl(oxo)-λ^5-phosphanyl

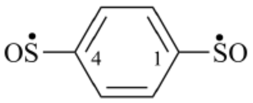
$CH_3\text{-}\dot{C}S$
ethanethioyl (PIN)
1-sulfanylideneethyl
1-thioxoethyl

$CH_3\text{-}CH_2\text{-}CH_2\text{-}\dot{C}(=NH)$

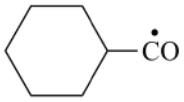
butanimidoyl (PIN)
1-iminobutyl



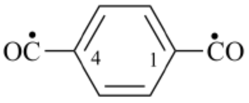
benzoyl (PIN)
benzenecarbonyl



benzene-1,4-disulfinyl (PIN)
(1,4-phenylene)bis(oxo-λ^4-sulfanyl)



cyclohexanecarbonyl (PIN)
cyclohexyl(oxo)methyl



benzene-1,4-dicarbonyl (PIN)
terephthaloyl
(1,4-phenylene)bis(oxomethyl)

P-71.3.2 A radical derived formally by the removal of hydrogen atoms from an amine, imine, or amide characteristic group is named by adding the appropriate cumulative suffix ‘-yl’ or ‘-ylidene’ to the basic suffix as shown here. This method is preferred to that using parent such as ‘azanyl’, and ‘nitrene’, or the functional modifier ‘imidyl’ in functional class nomenclature.

Table 7.2 Suffixes for Radicals of Amines, Imines and Amides

$-NH_2$	amine (preselected suffix)	$-\dot{N}H$	aminyl (preselected suffix)
		$-N^{2\bullet}$	aminylidene (preselected suffix)
$=NH$	imine (preselected suffix)	$=N\bullet$	iminyl (preselected suffix)
$-(C)O\text{-}NH_2$	amide (preferred suffix)	$-(C)O\text{-}\dot{N}H$	amidyl (preferred suffix)
		$-(C)O\text{-}N^{2\bullet}$	amidylidene (preferred suffix)
$-CO\text{-}NH_2$	carboxamide (preferred suffix)	$-CO\text{-}\dot{N}H$	carboxamidyl (preferred suffix)
		$-CO\text{-}N^{2\bullet}$	carboxamidylidene (preferred suffix)

Examples:

$CH_3\text{-}\dot{N}H$

methanaminyl (PIN)
methylazanyl
methylaminyl
(traditionally: methylamino)

$\overset{3}{C}H_3\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}H{=}N^{\bullet}$

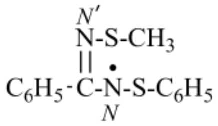
propan-1-iminyl (PIN)
propylideneazanyl

$C_6H_5\text{-}\dot{N}H$

benzenaminyl (PIN)
phenylaminyl
phenylazanyl
(traditionally: phenylamino)
(not anilino)

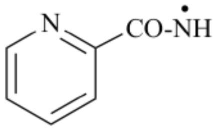
$(CH_3)_3P=N^•$
trimethyl-λ^5-phosphaniminyl (PIN)
trimethylphosphane imidyl

$HCO\text{-}\dot{N}H$
formamidyl (PIN)
formylazanyl
formylaminyl

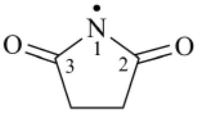


$$\begin{array}{l} \quad\;\; N' \\ \quad\;\; N\text{-}S\text{-}CH_3 \\ \quad\;\; \| \\ C_6H_5\text{-}C\text{-}\dot{N}\text{-}S\text{-}C_6H_5 \\ \qquad\quad\;\; N \end{array}$$

N′-(methylsulfanyl)-*N*-(phenylsulfanyl)benzenecarboximidamidyl (PIN)



pyridine-2-carboxamidyl (PIN)



2,5-dioxopyrrolidin-1-yl (PIN)
succinimidyl

$C_6H_5\text{-}N^{2•}$
benzenaminylidene (PIN)
phenylnitrene
phenylaminylene

$CH_3\text{-}CO\text{-}N^{2•}$
acetamidylidene (PIN)
acetylnitrene
acetylaminylene

P-71.3.3 Polyamine, polyimine and polyamide radicals

Polyradicals with radical centres identically derived but located on two or more amine, imine, or amide characteristic groups are named in two ways:

(1) by using suffixes (see P-71.3.2) denoting the removal of one hydrogen atom from each characteristic group and the multiplying prefixes ‘bis-’, ‘tris-’, etc.;

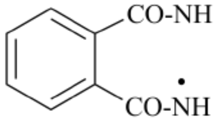
(2) by multiplicative nomenclature based on the parent radicals ‘azanyl’ and ‘azanylidene’.

In order to avoid any confusion, the name ‘aminyl’ is reserved for denoting the suffix in substitutive nomenclature; the parent radical ‘azanyl’ (not ‘aminyl’) is used in multiplicative nomenclature. Method (1) leads to preferred IUPAC names when a suffix described in P-71.3.2 is available.

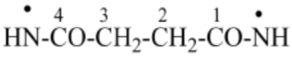
Examples:

$H\dot{N}\text{-}\overset{1}{C}H_2\text{-}\overset{2}{C}H_2\text{-}\dot{N}H$
(1) (ethane-1,2-diyl)bis(aminyl) (PIN)
(2) ethane-1,2-diylbis(azanyl)

$^•N=C=N^•$
(1) methanebis(iminyl) (PIN)
(2) methanediylidenebis(azanyl)



(1) benzene-1,2-bis(carboxamidyl) (PIN)
(2) (benzene-1,2-dicarbonyl)bis(azanyl)



$\mathrm{H}\overset{\bullet}{\mathrm{N}}\text{-}\overset{4}{\mathrm{C}}\mathrm{O}\text{-}\overset{3}{\mathrm{C}}\mathrm{H_2}\text{-}\overset{2}{\mathrm{C}}\mathrm{H_2}\text{-}\overset{1}{\mathrm{C}}\mathrm{O}\text{-}\overset{\bullet}{\mathrm{N}}\mathrm{H}$

(1) butanebis(amidyl) (PIN)
(2) butanedioylbis(azanyl)

$^{2\bullet}\mathrm{N\text{-}CO\text{-}[CH_2]_4\text{-}CO\text{-}N}^{2\bullet}$
(1) hexanebis(amidylidene) (PIN)
(2) hexanedioylbis(azanylidene)
hexanedioylbis(aminylidene)
hexanedioylbis(nitrene)

P-71.3.4 A radical derived formally by the removal of the hydrogen atom of a hydroxy group (or chalcogen analogue) of an acid or hydroxy characteristic group is named in two ways:

(1) additively, using the term ‘oxyl’ or ‘peroxyl’ derived from the terms ‘oxy’ or ‘peroxy’ (not dioxy);

(2) by substituting the parent radicals ‘oxidanyl’ (preselected name), for HO•, or ‘dioxidanyl’ (preselected name), for HOO•, by the appropriate substituent groups.

The names methoxyl, ethoxyl, propoxyl, butoxyl, *tert*-butoxyl, phenoxyl, and aminoxyl, which may be considered as contractions of the systematically formed names, such as methanyloxyl or methyloxyl, are retained and are preferred IUPAC names (see P-63.2.2.2 for names such as methoxy, ethoxy, etc.).

Method (1) generates preferred IUPAC names.

Examples:

$\mathrm{CH_3\text{-}O}\bullet$
(1) methoxyl (PIN)
(2) methyloxidanyl

$\mathrm{ClCH_2\text{-}CO\text{-}O}\bullet$
(1) (chloroacetyl)oxyl (PIN)
chloroacetoxyl
(2) (chloroacetyl)oxidanyl

$\mathrm{H_2N\text{-}O}\bullet$
aminoxyl (preselected name;
a contraction of aminooxyl)

$\mathrm{(ClCH_2)_2N\text{-}O}\bullet$
(1) bis(chloromethyl)aminoxyl (PIN)
(2) [bis(chloromethyl)amino]oxidanyl

$\mathrm{CH_3\text{-}[CH_2]_4\text{-}CO\text{-}O\text{-}O}\bullet$
(1) hexanoylperoxyl (PIN)
(2) hexanoyldioxidanyl

$\mathrm{CH_3\text{-}[CH_2]_3\text{-}O}\bullet$
(1) butoxyl (PIN)
(2) butyloxidanyl

$\mathrm{CH_3\text{-}[CH_2]_2CO\text{-}O}\bullet$
(1) butanoyloxyl (PIN)
(2) butanoyloxidanyl

Chalcogen analogues are named on the basis of preselected parent radical names, such as ‘sulfanyl’, ‘selanyl’, ‘disulfanyl’, etc.

Examples:

$\mathrm{C_6H_5\text{-}S}\bullet$
phenylsulfanyl (PIN)
(not benzenesulfenyl;
sulfenic acids are no longer recognized; see P-56.2)

$\mathrm{CH_3\text{-}Se}\bullet$
methylselanyl (PIN)

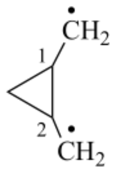
$\mathrm{CH_3\text{-}C(CH_3)_2\text{-}SS}\bullet$
tert-butyldisulfanyl (PIN)
(2-methylpropan-2-yl)disulfanyl

$\mathrm{ClCH_2}$-CS-S•
(chloroethanethioyl)sulfanyl (PIN)

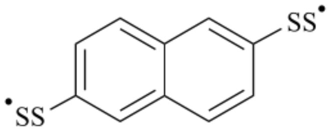
P-71.4 ASSEMBLIES OF PARENT RADICALS

Polyradicals with radical centers identically derived from the same parent hydride or the same characteristic group (except for polyacyl or polyamide radicals described in P-71.3.1 and P-71.3.3, respectively) but located in different parts of the structure are named, if possible, according to the principles for nomenclature of assemblies of identical units linked by multivalent substituents (see P-15.3).

Examples:

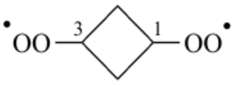


(cyclopropane-1,2-diyl)dimethyl (PIN)



(naphthalene-2,6-diyl)bis(disulfanyl) (PIN)

•O-C$\mathrm{(CH_3)_2}$-$\mathrm{CH_2}$-C$\mathrm{(CH_3)_2}$-O•
(1) (2,4-dimethylpentane-2,4-diyl)bis(oxyl) (PIN)
(1,1,3,3-tetramethylpropane-1,3-diyl)bis(oxyl)
(2) (2,4-dimethylpentane-2,4-diyl)bis(oxidanyl)



(1) (cyclobutane-1,3-diyl)bis(peroxyl) (PIN)
(2) (cyclobutane-1,3-diyl)bis(dioxidanyl)

P-71.5 PREFIXES DENOTING RADICALS

The presence of a radical center in a substituent that is to be cited as a prefix is expressed in two ways:

(1) by using the prefix ‘ylo’ that indicates the subtraction of a hydrogen atom from a substituent group, for example ‘–ylomethyl’ for –$\mathrm{CH_2}$•;

(2) by concatenation of prefixes, for example ‘oxylcarbonyl’ for –CO-O•.

This prefix is a nondetachable prefix, attached to the parent substituent prefix, which is formed by usual methods. The presence of two or more radical centers in a substituent cited as a prefix or the removal of two or more hydrogen atoms from a substituent cited as prefix is indicated by the appropriate multiplying prefix, ‘di’, ‘tri’, etc.

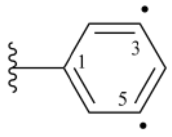
Examples:

$-\overset{\bullet}{\mathrm{C}}\mathrm{H_2}$
ylomethyl (preferred prefix)

–O•
ylooxidanyl (preselected prefix)
ylooxy
(not ylohydroxy)

$-\overset{\bullet}{\mathrm{C}}\mathrm{=O}$
yloformyl (preferred prefix)

–CO-O•
oxylcarbonyl (preferred prefix)
(ylooxidanyl)formyl

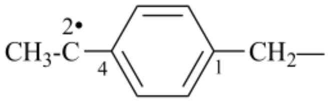


3,5-diylophenyl (preferred prefix)

$-\dot{N}H$

yloamino (preselected prefix)

yloazanyl



[4-(1,1-diyloethyl)phenyl]methyl (preferred prefix)

P-71.6 ORDER OF CITATION AND SENIORITY OF SUFFIXES ‘YL’, ‘YLIDENE’, AND ‘YLIDYNE’

The suffixes ‘yl’, ‘ylidene’, and ‘ylidyne’ are cited in that order in a name, if applicable; lowest locants are assigned to radicals as a set, then in the order ‘yl’, ‘ylidene’ and ‘ylidyne’. The order of citation is identical to that used for naming substituent groups (see P-29.3.2.2).

Example:

$\bullet CH_2\text{-}CH^{2\bullet}$

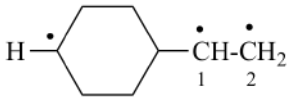
ethan-1-yl-2-ylidene (PIN)

P-71.7 CHOICE OF PARENT RADICAL

When a choice of a parent radical is necessary, the following criteria are applied, in the order given, until a decision is reached.

(a) Parent with the maximum number of radical centers of any kind in a single parent structure:

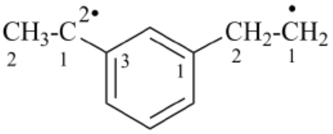
Example:



1-(4-ylocyclohexyl)ethane-1,2-diyl (PIN)
[not 4-(1,2-diyloethyl)cyclohexyl;
ethane has two radical centres, cyclohexane only has one]

(b) Parent with the maximum number of ‘-yl’ radical centers, then -ylidene radical centers;

Example:



2-[3-(1,1-diyloethyl)phenyl]ethyl (PIN)
{not 1-[3-(2-yloethyl)phenyl]ethylidene;
ethyl is senior to ethylidene}

(c) Parent with the maximum number of radical centers at the skeletal atom first cited in the seniority order of classes: N > P > As > Sb > Bi > Si > Ge > Sn > Pb > B > Al > Ga > In > Tl > O > S > Se > Te > C (see P-44.1.2)

The seniority order for radicals is now the order of seniority of classes rather than the order of skeletal replacement (‘a’) prefixes as used in RC-81.3.3.2, ref. 3.

Example:

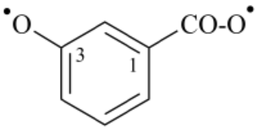
$\bullet CH_2\text{-}C(CH_3)_2\text{-}O\bullet$

(2-methyl-1-ylopropan-2-yl)oxyl (PIN)
(1,1-dimethyl-2-yloethyl)oxidanyl
(not 2-methyl-2-ylooxidanylpropyl;
oxyl is senior to propyl)

(d) Further choice, if necessary, is made by giving priority to the corresponding suffixes (see Table 4.4) and by using the general seniority order of classes (see P-41) and parent structures (see P-44). .

(1) maximum number of radical centers according to the order of suffixes (see P-33).

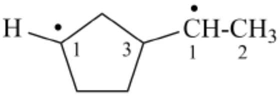
Example:



[3-(ylooxidanyl)benzoyl]oxyl (PIN)
[3-(ylooxidanyl)benzoyl]oxidanyl
{not 3-[(ylooxidanyl)carbonyl]phenoxyl;
ylooxidanyl is senior to phenoxyl}

(2) rings are senior to chains

Example:



3-(1-yloethyl)cyclopentyl (PIN)
[not 1-(3-ylocyclopentyl)ethyl;
cyclopentyl is senior to ethyl]

P-72 ANIONS

P-72.2 Anions formed by removal of hydrons
P-72.4 Skeletal replacement nomenclature
P-72.6 Anionic centers in both parent compounds and substituent groups
P-72.8 The suffixes 'ide' and 'uide' and the λ-convention

P-72.1 GENERAL METHODOLOGY

Anions are named in two ways:

(1) by using suffixes and endings;

(2) by functional class nomenclature.

Method (1) leads to preferred IUPAC names. Some names and some contracted names are retained as preferred IUPAC names and for use in general nomenclature.

The following suffixes are used:

'ide' (preferred suffix; corresponding to removal of a hydron, H^+),

'uide' (preferred suffix; corresponding to the addition of a hydride ion, H^-),

'elide' (preferred suffix; corresponding to the addition of an electron)

The endings 'ate' and 'ite' are used to indicate removal of a hydron from the –OH group of acids and hydroxy compounds.

Functional class nomenclature is based on the class name 'anion' in association with the name of the corresponding radical (not necessarily the name of the corresponding substituent group).

P-72.2 ANIONS FORMED BY REMOVAL OF HYDRONS

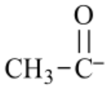
P-72.2.2 Systematic nomenclature

P-72.2.1 Functional class nomenclature

Functional class nomenclature can be used, in general nomenclature, to describe anionic compounds. An anion that can be considered as derived formally by adding an electron to a radical may also be named by adding the class name 'anion' as a separate word to the name of the substituent group. The names are formed by using the names of corresponding radicals (not necessarily the name of substitutent groups) and the class name 'anion' as a separate word. The multiplying prefixes 'di', 'tri', etc., are added to the class name to denote multiple anions. This type of nomenclature is limited to anions having anionic centers in the same structure. Systematic names (see P-72.2.2) are preferred IUPAC names.

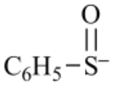
Examples:

H_3C^- methyl anion
methanide (PIN)



$CH_3{-}\overset{\overset{\large O}{||}}{C}{}^{-}$

acetyl anion
1-oxoethan-1-ide (PIN)

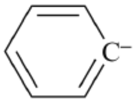


$C_6H_5{-}\overset{\overset{\large O}{||}}{S}{}^{-}$

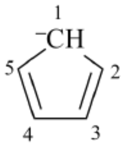
benzenesulfinyl anion
oxo(phenyl)-λ^4-sulfanide (PIN)

$CH_3\text{-}NH^-$
methanaminyl anion
methanaminide (PIN)

$(C_6H_5)_2C^{2-}$
diphenylmethylidene dianion
diphenylmethanediide (PIN)



phenyl anion
benzenide (PIN)



cyclopenta-2,4-dien-1-yl anion
cyclopenta-2,4-dien-1-ide (PIN)
cyclopentadienide (see P-76)

P-72.2.2 Systematic nomenclature

P-72.2.2.1 Anions derived from parent hydrides and their derivatives

An anion derived formally by the removal of one or more hydrons from any position of a neutral parent hydride is preferably named by using the suffix '-ide', with elision of the final letter 'e' of the parent hydride, if any. Numerical prefixes 'di', 'tri', etc. are used to denote multiplicity; locants identify positions of the negative charges.

The name 'acetylide', for $^-C{\equiv}C^-$, is retained for general use only.

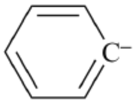
Examples:

$(NC)_3C^-$
tricyanomethanide (PIN)

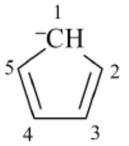
$(C_6H_5)_2C^{2-}$
diphenylmethanediide (PIN)

$(CH_3)_2P^-$
dimethylphosphanide (PIN)
dimethylphosphinide

$HC{\equiv}Si^-$
methylidynesilanide (PIN)



benzenide (PIN)



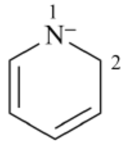
cyclopenta-2,4-dien-1-ide (PIN)
cyclopentadienide (see P-76)

$^-C{\equiv}C^-$
ethynediide (PIN)
acetylide

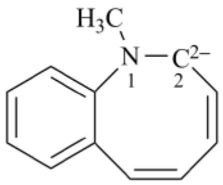
P-72.2.2.1.1 ‘Added indicated hydrogen’ for anions of mancude ring systems

An anionic center at a position in a mancude parent hydride where there is an insufficient number of hydrogen atoms to apply directly recommendations for the use of ‘ide’ given in P-72.2.2.1 is derived formally from a dihydro derivative of the cyclic parent hydride. Such an anion can also be described by applying the principle of ‘added indicated hydrogen’ (see P-14.7). In this method the ‘hydro’ derivative is described by specifying the hydrogen atom of a dihydro pair that remains after the anionic center is created by citing in italic capital *H* and the locant of the skeletal atom at which the hydrogen atom resides, both enclosed in a set of parentheses and inserted into the name of the corresponding parent hydride immediately after the locant for the anionic center. Names formed by the ‘added indicated hydrogen’ method are preferred IUPAC names (see P-58.2).

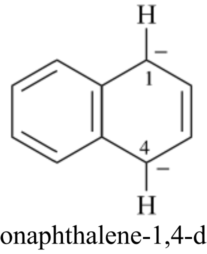
Examples:



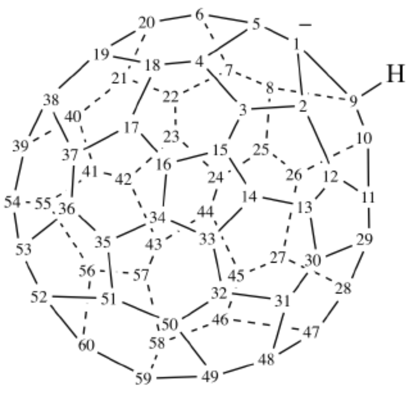
pyridin-1(2*H*)-ide (PIN)
1,2-dihydropyridine-1-ide



1-methyl-1-benzazocine-2,2(1*H*)-diide (PIN)
1-methyl-1,2-dihydro-1-benzazocine-2,2-diide



1,4-dihydronaphthalene-1,4-diide (PIN)



(C_{60}-I_h)[5,6]fulleren-1(9*H*)-ide (PIN)
1,9-dihydro(C_{60}-I_h)[5,6]fulleren-1-ide

P-72.2.2.2 Anions derived from characteristic groups are assigned IUPAC preferred names that are retained names or derived as follows:

(1) for acids, alcohols and amines by modifying the normally used in substitutive nomenclature:

(a) the endings ‘ate’ or ‘ite’ to name anions derived from acids;

(b) the ending ‘ate’ to name anions derived from alcohols,

(c) the suffix ‘aminide’ (formed by adding ‘ide’ to the suffix of the corresponding amine with elision of the final ‘e’ of ‘amine’, i.e., ‘amin(e) + ide’) to name anions derived from amines where the negative charge is on the nitrogen atom;

(2) by the appropriate preselected anionic parent names in the case of other characteristic groups, such as ‘azanide’ for NH_2^-, ‘azanediide’ for NH^{2-}, ‘oxidanide’ for HO^-.

(3) amides, hydrazides and imides are not named directly by method (1), as are amines and imines; the reason being that there could be real ambiguity to have the suffix ‘ide’ used at the end of names such as amide, hydrazides, etc.

Method (2) generates preferred names. Also, the name ‘amide’, which may be used in general nomenclature to designate the parent anion NH_2^-, would result in a certain degree of ambiguity. However, the use of parents ‘azanide’ and ‘azanediide’ eliminates all possible ambiguity.

P-72.2.2.2.1 Anions derived from acids
P-72.2.2.2.2 Anions derived from hydroxy compounds
P-72.2.2.2.3 Anions derived from amines and imines
P-72.2.2.2.4 Anions derived from other characteristic groups

P-72.2.2.2.1 Anions derived from acids

P-72.2.2.2.1.1 The preferred IUPAC name of anions formed by the removal of a hydron from the chalcogen atom (O, S, Se, and Te) of an acid or peroxyacid characteristic group or functional parent compound is formed by replacing the ‘ic acid’ or ‘ous acid’ ending of the acid name by ‘ate’ or ‘ite’, respectively. Names of acids are described in Sections P-65 and P-67.

This is a change from recommendation RC-83.1.6 (ref. 3) in which peroxyacids and their chalcogen analogues modified by functional replacement were named on the basis of an anionic parent hydride.

Examples:

$CH_3CO\text{-}O^-$
acetate (PIN)

$CH_3\text{-}CH_2\text{-}CO\text{-}O\text{-}O^-$
propaneperoxoate (PIN)

$CH_3\text{-}CS\text{-}O\text{-}O^-$
ethaneperoxothioate (PIN)
(ethanethioyl)dioxidanide
(thioacetyl)dioxidanide

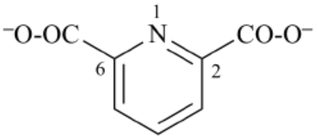
$CH_3\text{-}CO\text{-}O\text{-}S^-$
ethane(*OS*-thioperoxoate) (PIN)
(acetyloxy)sulfanide
(not acetoxysulfanide)

$CH_3\text{-}CH_2\text{-}CO\text{-}S^- \leftrightarrow CH_3\text{-}CH_2\text{-}CS\text{-}O^-$
propanethioate (PIN)

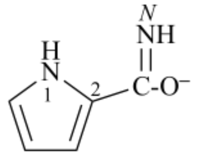
$CH_3\text{-}CO\text{-}S^- \leftrightarrow CH_3\text{-}CS\text{-}O^-$
ethanethioate (PIN)

$C_6H_5\text{-}SO_2\text{-}O^-$
benzenesulfonate (PIN)

$(C_6H_5\text{-}CH_2)_2P\text{-}O^-$
dibenzylphosphinite (PIN)



pyridine-2,6-dicarboxylate (PIN)



1*H*-pyrrole-2-carboximidate (PIN)

P-72.2.2.2.1.2 Acid esters of organic acids

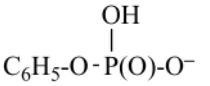
Preferred IUPAC names of acid esters of 'organic acids' as discussed in P-65 are formed substitutively (see P-65.6.3.3.5) rather than by the method of 'hydrogen salts'. Preferred IUPAC names of acid esters of inorganic acids as discussed in P-67.1.3.2 are formed by the method of 'hydrogen salts'; see P-65.6.2.3 and P-65.6.3.3.5.

Examples:

$HOOC\text{-}[CH_2]_4\text{-}CO\text{-}O^-$
5-carboxypentanoate (PIN)
hydrogen hexanedioate

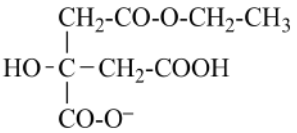
$C_6H_5\text{-}P(O)(OH)\text{-}O^-$
hydrogen phenylphosphonate (PIN)
[not hydroxy(phenyl)phosphinate;
phosphonic acid is senior to phosphinic acid]

$CH_3\text{-}CH_2\text{-}O\text{-}CO\text{-}CH_2\text{-}CH_2\text{-}CO\text{-}O^-$
4-ethoxy-4-oxobutanoate (PIN)
ethyl butanedioate
ethyl succinate



$$C_6H_5\text{-}O\text{-}\overset{\overset{\displaystyle OH}{|}}{P}(O)\text{-}O^-$$

phenyl hydrogen phosphate (PIN)



$$HO\text{-}\underset{\underset{\displaystyle CO\text{-}O^-}{|}}{\overset{\overset{\displaystyle CH_2\text{-}CO\text{-}O\text{-}CH_2\text{-}CH_3}{|}}{C}}\text{-}CH_2\text{-}COOH$$

2-(carboxymethyl)-4-ethoxy-2-hydroxy-4-oxobutanoate (PIN)
4-ethyl 2-(carboxymethyl)-2-hydroxybutanedioate
3-ethyl 1-hydrogen citrate
4-hydrogen 2-(2-ethoxy-2-oxoethyl)-2-hydroxybutanedioate

P-72.2.2.2.2 Anions derived from hydroxy compounds

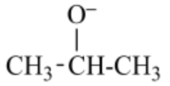
An anion formed by subtracting a hydron from the chalcogen atom of a hydroxy characteristic group, or a chalcogen analogue, that can be expressed by a suffix such as 'ol', 'thiol', 'peroxol', etc., is preferably named by using suffixes 'olate', 'thiolate', 'peroxolate', etc., formed by addition of the ending 'ate' to the suffixes 'ol', 'thiol', 'peroxol', etc. The multiplying prefixes 'bis', 'tris', etc. are used before these suffixes, to avoid any ambiguity.

The retained names hydroxide, for HO^-, and hydroperoxide, for HOO^-, are preseleted names but cannot be substituted; thus, for $CH_3\text{-}O^-$ and $CH_3\text{-}OO^-$ the names are methoxide or methanolate or methyloxidanide, and methaneperoxolate or methyldioxidanide, respectively.

The traditional names methoxide, ethoxide, propoxide, butoxide, *tert*-butoxide, phenoxide (but not isopropoxide), and aminoxide, for $CH_3\text{-}O^-$, $C_2H_5\text{-}O^-$, $C_3H_7\text{-}O^-$, $C_4H_9\text{-}O^-$, $(CH_3)_3C\text{-}O^-$, $C_6H_5\text{-}O^-$, and $H_2N\text{-}O^-$, are retained as preferred IUPAC names or preselected name. *tert*-Butoxide cannot be substituted. Isopropoxide, $(CH_3)_2CH\text{-}O–$, is retained for general nomenclature but cannot be substituted.

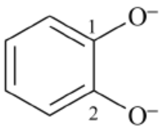
Examples:

$CH_3\text{-}O^-$
methoxide (PIN)
methanolate

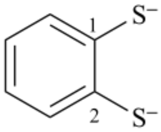


$$CH_3\text{-}\overset{\overset{\displaystyle O^-}{|}}{C}H\text{-}CH_3$$

propan-2-olate (PIN)
isopropoxide



benzene-1,2-bis(olate) (PIN)
(not pyrocatecholate)

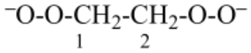


benzene-1,2-bis(thiolate) (PIN)

$(CH_3)_2N\text{-}O^-$
dimethylaminoxide (PIN)
(dimethylamino)oxidanide

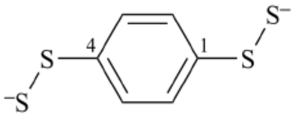
$CH_3\text{-}O\text{-}O^-$
methaneperoxolate (PIN)
methyldioxidanide

$CH_3\text{-}CH_2\text{-}S\text{-}O^-$
ethane(*SO*-thioperoxolate) (PIN)
(ethylsulfanyl)oxidanide
(not ethanesulfenate;
sulfenic acids are no longer recommended; see P-56.2)

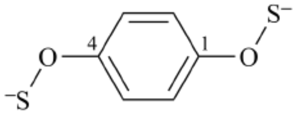


$${}^{-}O\text{-}O\text{-}\underset{1}{CH_2}\text{-}\underset{2}{CH_2}\text{-}O\text{-}O^{-}$$

ethane-1,2-bis(peroxolate) (PIN)
(ethane-1,2-diyl)bis(dioxidanide)



benzene-1,4-bis(dithioperoxolate) (PIN)
(1,4-phenylene)bis(disulfanide)



benzene-1,4-bis(*OS*-thioperoxolate) (PIN)
(1,4-phenylene)bis(oxy)bis(sulfanide)

P-72.2.2.2.3 Anions derived from amines and imines

Amines and imines having one negative charge on each nitrogen atom are named by using the suffixes ‘aminide’ and ‘iminide’, formed by the addition of the suffix ‘ide’ to the suffix ‘amine’ or ‘imine’, respectively; the prefix ‘bis-’ is used to indicate two aminide suffixes. The resulting names are preferred IUPAC names. When two negative charges are present on the nitrogen atom of an amine, the suffix ‘aminediide’ is used to generate preferred IUPAC names. The retained names ‘amide’ and ‘imide’ for the anions H_2N^- and HN^{2-}, respectively, may be used as parent anions in general nomenclature.

The use of compound suffixes ‘aminide’, ‘iminide’ and ‘aminediide’ is a change from previous practice where parent anions H_2N^- and HN^{2-} were used to express amines and imines having negative charge(s).

Examples:

$CH_3\text{-}NH^-$
methanaminide (PIN)
methylamide

$C_6H_5\text{-}NH^-$
benzenaminide (PIN)
phenylamide

$H\bar{N}\text{-}\underset{1}{CH_2}\text{-}\underset{2}{CH_2}\text{-}\bar{N}H$
ethane-1,2-bis(aminide) (PIN)
(ethane-1,2-diyl)bis(amide)

$\overset{4}{CH_3}\text{-}\overset{3}{CH_2}\text{-}\overset{2}{CH_2}\text{-}\overset{1}{CH}{=}N^-$
butaniminide (PIN)

$(CH_3)_3P{=}N^-$
trimethyl-λ^5-phosphaniminide (PIN)

$CH_3\text{-}CH_2\text{-}N^{2-}$
ethanaminediide (PIN)
ethylazanediide
ethylimide

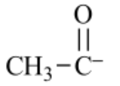
$C_6H_5\text{-}N^{2-}$
benzenaminediide (PIN)
phenylazanediide
phenylimide

P-72.2.2.2.4 Anionic centers on other characteristic groups

Anionic centers generated formally by the removal of hydrons from atoms of characteristic groups other than those considered in P-72.2.2.2.1, P-72.2.2.2.2, and P-72.2.2.2.3 are named on the basis of the corresponding anionic parent hydrides. Suffixes such as ‘amidide’ and ‘carboxamidide’ are not recommended.

Examples:

$(CH_3)_3C\text{-}O\text{-}O\text{-}O^-$
tert-butyltrioxidanide (PIN)
(2-methylpropan-2-yl)trioxidanide
(1,1-dimethylethyl)trioxidanide

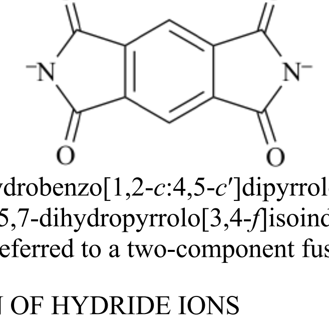

$CH_3\text{-}\overset{\overset{\displaystyle O}{||}}{C}{}^-$
1-oxoethan-1-ide (PIN)

$CH_3\text{-}CO\text{-}NH^-$
acetylazanide (PIN)
acetylamide

$CH_3\text{-}CO\text{-}\underset{2}{N}H\text{-}\underset{1}{N}^{2\bullet}$
acetylhydrazine-1,1-diide (PIN)
acetyldiazane-1,1-diide

$HO\text{-}NH^-$
hydroxyazanide (preselected name)
hydroxyamide

$HO\text{-}N^{2-}$
hydroxyazanediide (preselected name)
hydroxyimide


1,3,5,7-tetraoxo-5,7-dihydrobenzo[1,2-*c*:4,5-*c*′]dipyrrole-2,6(1*H*,3*H*)-diide (PIN)
(not 1,3,5,7-tetraoxo-5,7-dihydropyrrolo[3,4-*f*]isoindole-2,6(1*H*,3*H*)-diide;
a multiparent system is preferred to a two-component fused system, see P-25.3.5.3)

P-72.3 ANIONS FORMED BY ADDITION OF HYDRIDE IONS

Two methods are used to name anions formally derived by the addition of a hydride ion, H$^-$:

(1) the suffix 'uide' describes an anion formally derived by adding a hydride ion, H^-, to a parent hydride name; the multiplying prefixes 'di', 'tri', etc. indicating multiplicity;

(2) by adding the suffix 'ide' to a parent hydride in which the bonding number at the anionic site is higher than the standard bonding number and is expressed by the λ-convention; the net effect of which is the addition of a hydride ion, H^-, to the parent hydride with its standard bonding number (see P-72.2.2.1).

> In previous recommendations, the skeletal replacement prefix 'borata' was used to describe the addition of a hydride ion.

Method (1) leads to preferred IUPAC names.

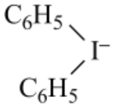
Examples:

$CH_3\text{-}\overline{Si}H_4$
methylsilanuide (PIN)

$(CH_3)_4B^-$
tetramethylboranuide (PIN)

$(CH_3)_4P^-$
tetramethylphosphanuide (PIN)
tetramethyl-λ^5-phosphanide
tetramethylphosphoranide

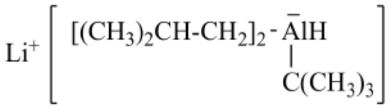
$C_6H_5\text{-}\overline{S}F_2$
difluoro(phenyl)sulfanuide (PIN)
difluoro(phenyl)-λ^4-sulfanide

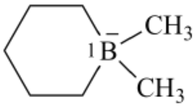

diphenyliodanuide (PIN)
diphenyl-λ^3-iodanide

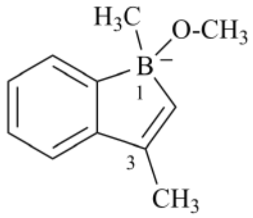
F_6I^-
hexafluoro-λ^5-iodanuide (preselected name)
hexafluoro-λ^7-iodanide

F_8Te^{2-}
octafluoro-λ^6-tellanediuide (preselected name)
octafluoro-λ^{10}-tellanediide

$Na^+\ (CH_3)_3\overline{B}H$
sodium trimethylboranuide (PIN)


$$Li^+\left[\begin{array}{l}[(CH_3)_2CH\text{-}CH_2]_2\text{-}\overline{Al}H\\ \qquad\qquad\qquad\qquad\quad |\\ \qquad\qquad\qquad\qquad C(CH_3)_3\end{array}\right]$$
lithium *tert*-butylbis(2-methylpropyl)alumanuide


1,1-dimethylborinan-1-uide (PIN)
(not 1,1-dimethyl-1-boratacyclohexane)


1-methoxy-1,3-dimethyl-1*H*-1-benzoborol-1-uide (PIN)
(not 1-methoxy-1,3-dimethyl-1-borataindene)

P-72.4 SKELETAL REPLACEMENT NOMENCLATURE

Anionic centers in parent hydrides are named by two methods using the principles of skeletal replacement (‘a’) nomenclature described in Section P-15.4:

(1) by forming the name of the neutral compound according to skeletal replacement (‘a’) nomenclature and using the suffixes ‘ide’ and ‘uide’ to describe the anionic centers;

(2) by adding anionic skeletal replacement (‘a’) prefixes formed by adding the suffixes ‘ida’ and ‘uida’ to the name of the corresponding mononuclear parent hydride, with elision of the final letter ‘e’; these replacement prefixes indicate an anionic center having a bonding number one lower or one higher, respectively, than the bonding number of the corresponding neutral mononuclear parent hydride.

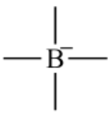
Method (1) results in preferred IUPAC names. In other words, names that do not require designation of skeletal heteroatoms in nonstandard valence states using the λ-convention are preferred (see P-72.3).

Skeletal replacement (‘a’) prefixes ending in ‘ata’, for example ‘borata’, are no longer recognized.

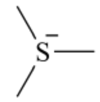
Examples:

$-\overline{P}-$

phosphanida (preselected name)

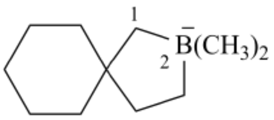


boranuida (preselected name)
(not borata)

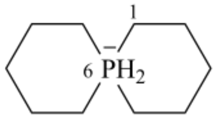


sulfanuida (preselected name)

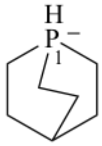
Examples:



2,2-dimethyl-2-boraspiro[4.5]decan-2-uide (PIN)
2,2-dimethyl-2-boranuidaspiro[4.5]decane
(not 2,2-dimethyl-2-borataspiro[4.5]decane)



6λ^5-phosphaspiro[5.5]undecan-6-uide (PIN)
6λ^5-phosphanuidaspiro[5.5]undecane
(not 6-phosphataspiro[5.5]undecane)



1-phosphabicyclo[2.2.2]octan-1-uide (PIN)
1-phosphanuidabicyclo[2.2.2]octane
1λ^5-phosphabicyclo[2.2.2]octan-1-ide
1λ^5-phosphanidabicyclo[2.2.2]octane

P-72.5 MULTIPLE ANIONIC CENTERS

Multiple anionic centers are named by several methods in accordance with the previous rules.

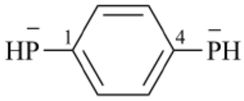
P-72.5.1 Assemblies of parent anions
P-72.5.2 ‘Ide’ and ‘uide’ centers in the same parent hydride
P-72.5.3 Anionic characteristic groups on anionic parent hydrides

P-72.5.1 Assemblies of parent anions

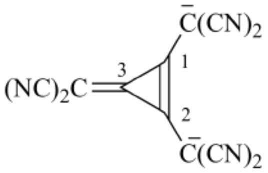
P-72.5.1.1 Assemblies derived from parent anions

Anionic compounds with anionic centers derived from the same parent hydride, but located in different parts of a structure, are named, if possible, according to the principles of multiplicative nomenclature (see P-15.3), using the multiplying prefixes ‘bis’, ‘tris’, etc., where necessary.

Examples:



(1,4-phenylene)bis(phosphanide) (PIN)



[3-(dicyanomethylidene)cycloprop-1-ene-1,2-diyl]bis(dicyanomethanide) (PIN)

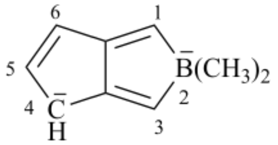
$H\bar{N}\text{-CO-CH}_2\text{-CH}_2\text{-CO-}\bar{N}H$

butanedioylbis(azanide) (PIN)
butanedioylbis(amide)

P-72.5.2 ‘Ide’ and ‘uide’ centers in the same parent hydride

Anionic compounds with two or more anionic centers in the same parent hydride structure, at least one of which is derived formally by removal of a hydron from a skeletal position and one by adding a hydride ion at another position, are named by adding the suffix ‘-ide’, then the suffix ‘-uide’ to the name of the parent hydride, with elision of the final letter ‘e’ of the parent hydride and of the suffix ‘-ide’. Each suffix is preceded, where necessary, by the appropriate multiplying prefix. Where there is a choice, low locants of the parent hydride are assigned first to the anionic centers regardless of the kind and then to ‘-uide’ anionic centers.

Example:

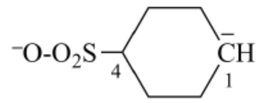


2,2-dimethyl-2,4-dihydrocyclopenta[*c*]borol-4-id-2-uide (PIN)

P-72.5.3 Anionic characteristic groups on anionic parent hydrides

Polyanions with anionic centers both in the parent hydride part of the structure and on a characteristic group that may be expressed as an anionic suffix are named by adding the anionic suffix to the name of a parent anion formed according to Rules P-72.2.2.1 and P-72.2.2.2. Where there is a choice, low locants are assigned to the anionic skeletal atoms.

Examples:



cyclohexan-1-ide-4-sulfonate (PIN)

$^{-}\text{O-CO-CH}_2\text{-CH}_2\text{-C}{\equiv}\text{C}^{-}$

pent-1-yn-1-id-5-oate (PIN)

P-72.6 ANIONIC CENTERS IN BOTH PARENT COMPOUNDS AND SUBSTITUENT GROUPS

When anionic centers are not in the same parent structure, one anion must be chosen as the parent anion and the other expressed as anionic substituent group(s).

P-72.6.1 Prefixes for anionic centers derived from acid characteristic groups
P-72.6.2 Prefixes for anionic chalcogens
P-72.6.3 Systematically formed prefixes that include anionic center(s)

P-72.6.1 Prefixes for anionic centers derived from acid characteristic groups

Substituent anions derived from acid characteristic groups by removal of a hydron from all hydroxy, thiol, etc. groups or a chalcogen analogue, and that are attached to the parent structure by a single bond are named by prefixes formed by changing the ending ‘ate’ in the name of the anionic suffix to ‘ato’.

Examples:

$-CO\text{-}O^-$
carboxylato (preferred prefix)

$-SO_2\text{-}O^-$
sulfonato (preselected prefix)

$-P(O)(O^-)_2$
phosphonato (preselected prefix)

$-As(O)(O^-)_2$
arsonato (preselected prefix)

P-72.6.2 Prefixes for anionic chalcogens

These prefixes are derived from the names oxide, sulfide, selenide, and telluride by changing the final letter ‘e’, to ‘o’.

Examples:

$-O^-$
oxido (preselected prefix)

$-S^-$
sulfido (preselected prefix)

P-72.6.3 Systematically formed prefixes that include anionic center(s)

These prefixes are formed by adding the cumulative suffixes ‘yl’ or ‘ylidene’ to the name of the parent anion, with elision of the final letter ‘e’ in the name of the parent anion. Multiplying prefixes ‘di’, ‘tri’, etc, are used to denote multiplicity of free valences. Where there is a choice, low locants are assigned to the free valences.

Examples:

$-CH_2^-$
methanidyl (preferred prefix)

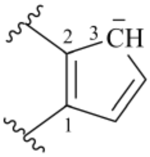
$-NH^-$
azanidyl (preselected prefix)
amidyl

$-N^{2-}$
azanediidyl (preselected prefix)

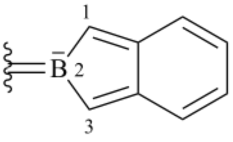
$-BH_3^-$
boranuidyl (preselected prefix)

$=N^-$
azanidylidene (preselected prefix)
amidylidene

$-S\text{-}S^-$
disulfanidyl (preselected prefix)



cyclopenta-1,4-dien-3-ide-1,2-diyl (preferred prefix)



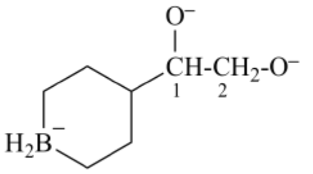
2*H*-2-benzoborol-2-uid-2-ylidene (preferred prefix)

P-72.7 CHOICE OF AN ANIONIC PARENT STRUCTURE

When necessary, a parent anionic structure must be chosen by applying the following criteria in order until a definitive choice is achieved:

(a) parent with the maximum number of anionic centers, including anionic suffixes;

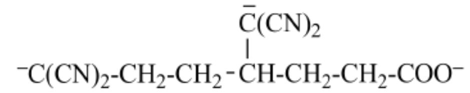
Example:



1-(borinan-1-uid-4-yl)ethane-1,2-bis(olate) (PIN)
[not 4-(1,2-dioxidoethyl)borinan-1-uide;
two anionic centre is senior to one]

(b) parent with the maximum number of 'uide' and 'ide' anionic centers ;

Example:



$$^{-}C(CN)_2\text{-}CH_2\text{-}CH_2\text{-}\overset{\bar{C}(CN)_2}{\overset{|}{C}H}\text{-}CH_2\text{-}CH_2\text{-}COO^{-}$$

2-(2-carboxylatoethyl)-1,1,5,5-tetracyanopentane-1,5-diide (PIN)
[not 1,1-dicyano-4-(dicyanomethanidyl)heptan-1-id-7-oate;
diide is senior to idoate]

(c) parent with the maximum number of 'uide' centers;

Example:

$$\bar{P}H\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}H_2\text{-}\bar{As}H_3$$

(2-phosphanidylethyl)arsanuide (PIN)
[not (2-arsanuidylethyl)phosphanide]

(d) parent with the maximum number of senior anionic centers first cited in the seniority order of classes: N > P > As > Sb > Bi > Si > Ge > Sn > Pb > B > Al > Ga > In > Tl > O > S > Se > Te > C (see P-44.1.2);

> The seniority order for anions is now the order of seniority of classes rather than the order of skeletal replacement ('a') prefixes as used in RC-83.4.7.4, ref. 3.

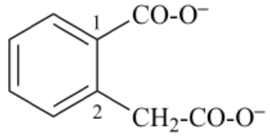
Example:

$$\bar{Si}H_2\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}H_2\text{-}\bar{P}H$$

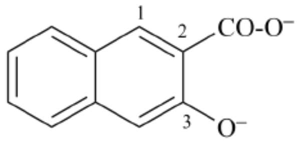
(2-silanidylethyl)phosphanide (PIN)
[not (2-phosphanidylethyl)silanide; P > Si]

(e) further choice, if necessary, is made by giving priority to corresponding suffixes (see Table 4.4) and by using the general seniority order of classes (see P-41) and parent structures (see P-44).

Examples:



2-(carboxylatomethyl)benzoate (PIN)
(ring senior to a chain)



3-oxidonaphthalene-2-carboxylate (PIN)
(carboxylate senior to olate)

P-72.8 THE SUFFIXES 'IDE' AND 'UIDE' AND THE λ-CONVENTION

P-72.8.1 The suffix 'uide' is preferred to the suffix 'ide' with a parent hydride named by the λ-convention.

Examples:

$$CH_3\text{-}\bar{Si}H_4$$

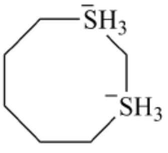
methylsilanuide (PIN)
methyl-λ^6-silanide

F_6I^-
hexafluoro-λ^5-iodanuide (preselected name)
hexafluoro-λ^7-iodanide

P-72.8.2 The suffix 'ide' is preferred to the suffix 'uide' involved with the λ-convention; the suffix 'ide' is also preferred over 'uide' when the λ-convention is involved in both anionic centers.

Examples:

H_3C^-
methanide (PIN)
λ^2-methanuide



1λ^6,3λ^6-dithiocane-1,3-diide (PIN)
1λ^4,3λ^4-dithiocane-1,3-diuide
(not 1λ^4,3λ^6-dithiocan-3-id-1-uide;
identical groups, if possible, must not be named differently within a name)

P-73 CATIONS

P-73.0 INTRODUCTION

For the purpose of organic nomenclature a cation is a molecular entity carrying at least one unit of positive charge formally derived from a parent hydride or parent compound by adding one or more hydrons, by the removal of one or more hydride ions, or a combination of these operations. An atom where a positive charge is considered to reside is called a cationic center. Cations with two or more cationic centers in the same structure are called dications, trications, etc.

P-73.1 Cationic compounds with cationic centers derived formally by the addition of hydrons
P-73.2 Cationic compounds with cationic centers derived formally by the removal of hydride ions
P-73.3 The λ-convention with the suffix 'ylium'
P-73.4 Skeletal replacement ('a') nomenclature for cations
P-73.5 Cationic compounds with multiple cationic centers
P-73.6 Cationic prefix names
P-73.7 Choice of a parent structure
P-73.8 The suffixes 'ium' and 'ylium' and the λ-convention

P-73.1 CATIONIC COMPOUNDS WITH CATIONIC CENTERS DERIVED FORMALLY BY THE ADDITION OF HYDRONS

P-73.1.1 Cationic centers in parent hydrides
P-73.1.2 Cationic centers on characteristic groups

P-73.1.1 Cations centers in parent hydrides

P-73.1.1.1 Retained names for monocationic mononuclear parent cations of the Group 15, 16, and 17 elements used only for general nomenclature.

A parent ion derived formally by adding one hydron to a mononuclear parent hydride of the nitrogen, chalcogen, and halogen families in its standard bonding state is named by adding the term 'onium' to a root for the element as indicated in Table 7.3. These cations are parent compounds; they can be substituted, but are used only in general nomenclature. For preferred IUPAC names see P-73.1.1.2.

Table 7.3 Retained names for the mononuclear parent cations of the Group 15, 16, and 17 elements

H_4N^+	ammonium	H_3O^+	oxonium	H_2F^+	fluoronium
H_4P^+	phosphonium	H_3S^+	sulfonium	H_2Cl^+	chloronium
H_4As^+	arsonium	H_3Se^+	selenonium	H_2Br^+	bromonium
H_4Sb^+	stibonium	H_3Te^+	telluronium	H_2I^+	iodonium
H_4Bi^+	bismuthonium				

Examples:

$(CH_3)_4N^+$
tetramethylammonium
tetramethylazanium
N,*N*,*N*-trimethylmethanaminium (PIN)

$Cl(CH_3)_3P^+$
chlorotri(methyl)phosphonium
chlorotri(methyl)phosphanium (PIN)

$(CH_3)_2\overset{+}{S}H$
dimethylsulfonium
dimethylsulfanium (PIN)

$CH_3\text{-}C{\equiv}O^+$
ethylidyneoxonium
ethylidyneoxidanium(PIN)

$(C_6H_5)_2I^+$
diphenyliodonium
diphenyliodanium (PIN)

$CH_3\text{-}\overset{+}{F}\text{-}Cl$
chloro(methyl)fluoronium
chloro(methyl)fluoranium (PIN)

P-73.1.1.2 General rule for systematically naming cationic centers in parent hydrides

A cation derived formally by adding one or more hydrons to any position of a neutral parent hydride (listed in Chapter P-2), or whose degree of hydrogenation has been modified (see P-31) is named by replacing the final letter ‘e’ of the parent hydride name, if any, by the suffix ‘ium’, preceded by multiplying prefixes ‘di’, ‘tri’, etc. to denote the multiplicity of identical cationic centers. These names for mononuclear cations derived from the mononuclear parent hydrides of the Group 15, 16, and 17 elements are the preferred IUPAC names and not those given in Table 7.3. When the hydron is not specifically localized the structure is enclosed in square brackets.

Examples:

${}^+CH_5$
methanium (PIN)

$[C_6H_7]^+$
benzenium (PIN)

H_4N^+
azanium (preselected name)
ammonium

H_4P^+
phosphanium (preselected name)
phosphonium

H_3S^+
sulfanium (preselected name)
sulfonium

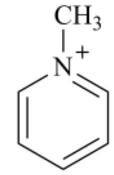
H_2Cl^+
chloranium (preselected name)
chloronium

$CH_3\text{-}\overset{+}{S}F_4$
tetrafluoro(methyl)-λ^4-sulfanium (PIN)
tetrafluoro(methyl)-λ^4-sulfonium

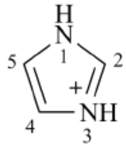
$(CH_3)_2N\text{-}\overset{+}{N}(CH_3)_3$
pentamethylhydrazinium (PIN)
pentamethyldiazanium

$CH_3\text{-}S\text{-}\overset{+}{S}(CH_3)\text{-}S\text{-}CH_3$
1,2,3-trimethyltrisulfan-2-ium (PIN)

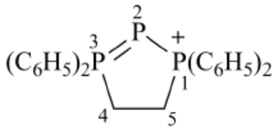
$Cl_2P\text{-}\overset{+}{P}(CH_3)_3$
2,2-dichloro-1,1,1-trimethyldiphosphan-1-ium (PIN)



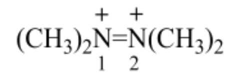
1-methylpyridin-1-ium (PIN)



1*H*-imidazol-3-ium (PIN)

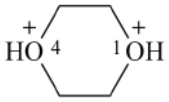


1,1,3,3-tetraphenyl-4,5-dihydro-1*H*-1,2,3λ^5-triphosphol-1-ium (PIN)

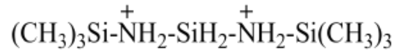


$(\mathrm{CH_3})_2\underset{1}{\overset{+}{\mathrm{N}}}=\underset{2}{\overset{+}{\mathrm{N}}}(\mathrm{CH_3})_2$

tetramethyldiazene-1,2-diium (PIN)



1,4-dioxane-1,4-diium (PIN)



$(\mathrm{CH_3})_3\mathrm{Si}\text{-}\overset{+}{\mathrm{N}}\mathrm{H_2}\text{-}\mathrm{SiH_2}\text{-}\overset{+}{\mathrm{N}}\mathrm{H_2}\text{-}\mathrm{Si(CH_3)_3}$

N,*N*′-bis(trimethylsilyl)silanebis(aminium) (PIN)

P-73.1.2 Cationic centers on characteristic groups

The principle applied in the naming of cationic centers on characteristic groups is that the largest neutral parent possible is used. It is applied particularly in the case of neutral compounds expressed by suffixes containing nitrogen (see Table 7.4, below). Other classes are named on the basis of the largest cationic parent hydride.

Table 7.4 Suffixes for cationic characteristic groups[1]

Neutral characteristic group suffix	Cationic characteristic group suffix
amide, carboxamide	amidium, carboxamidium
imide, carboximide	imidium, carboximidium
nitrile, carbonitrile	nitrilium, carbonitrilium
amine	aminium
imine	iminium

---

[1] When retained names of amides and nitriles used in general nomenclature imply the presence of two characteristic groups, for example succinonitrile, the corresponding cationic suffix denotes the addition of one hydron to each of the characteristic groups.

P-73.1.2.1 Cationic compounds derived from neutral compounds expressed by suffixes are named in two ways.

(1) Cationic suffixes derived from names of acids named by a suffix, amides, imides, nitriles, amines, and imines are formed by adding the suffix ‘ium’ to the basic suffix, as indicated in Table 7.4. These cationic suffixes are used with the multiplying prefixes ‘bis’, ‘tris’, etc. to denote multiplicity. Retained names, whether used as preferred IUPAC names or in general nomenclature (with the exception of ‘urea’, see P-73.1.2.2), are modified by adding the suffix ‘ium’ to the name of the neutral entity.

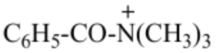
(2) by substituting cationic parent hydrides described in P-73.1.2 when no nitrogen atom is present.

Methods (1) and (2) are used to generate preferred IUPAC names as illustrated by the examples below.

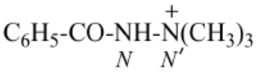
Examples:

$(CH_3)_4N^+$

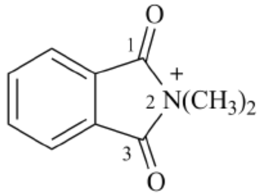
N,*N*,*N*-trimethylmethanaminium (PIN)
tetramethylammonium


$C_6H_5\text{-}CO\text{-}\overset{+}{N}(CH_3)_3$

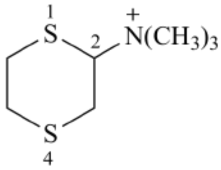
N,*N*,*N*-trimethylbenzamidium (PIN)
benzoyltri(methyl)ammonium


$C_6H_5\text{-}CO\text{-}\underset{N}{NH}\text{-}\underset{N'}{\overset{+}{N}}(CH_3)_3$

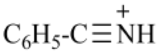
N′,*N*′,*N*′-trimethylbenzohydrazid-*N*′-ium (PIN)
2-benzoyl-1,1,1-trimethylhydrazinium
2-benzoyl-1,1,1-trimethyldiazan-1-ium



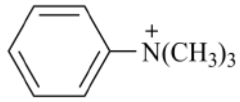
2,2-dimethyl-1,3-dioxo-2,3-dihydro-1*H*-isoindol-2-ium (PIN)
N,*N*-dimethylphthalimidium



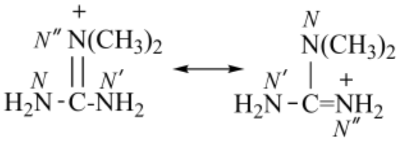
N,*N*,*N*-trimethyl-1,4-dithian-2-aminium (PIN)
(1,4-dithian-2-yl)tri(methyl)ammonium


$C_6H_5\text{-}C\equiv\overset{+}{N}H$

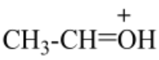
benzonitrilium (PIN)
benzylidyneammonium
benzylidyneazanium



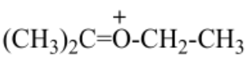
N,*N*,*N*-trimethylanilinium (PIN)
N,*N*,*N*-trimethylbenzenaminium
trimethyl(phenyl)ammonium



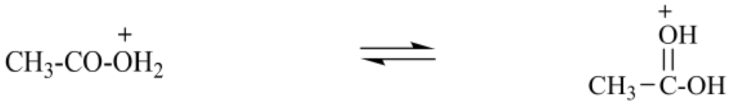
N,*N*-dimethylguanidinium (PIN)
(locants ‘*N*,*N*’ are lower than ‘*N*′,*N*′’ in designating these resonance forms)


$CH_3\text{-}CH{=}\overset{+}{O}H$

ethylideneoxidanium (PIN)
ethylideneoxonium


$(CH_3)_2C{=}\overset{+}{O}\text{-}CH_2\text{-}CH_3$

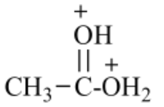
ethyl(propan-2-ylidene)oxidanium (PIN)
ethyl(propan-2-ylidene)oxonium



acetic acidium

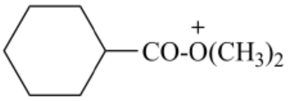
acetyloxidanium (PIN)
(1-hydroxyethylidene)oxidanium (PIN)

Note: The term ‘acidium’ covers the two tautomeric structures; individual tautomers are named systematically on the basis of the ‘oxidanium ion’.

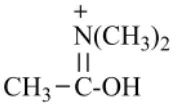


$$\begin{array}{l}\overset{+}{O}H\\ \|\\ CH_3-C\text{-}\overset{+}{O}H_2\end{array}$$

(1-oxidaniumylethylidene)oxidanium (PIN)
acetic acidodiium



(cyclohexanecarbonyl)di(methyl)oxidanium (PIN)
(cyclohexanecarbonyl)di(methyl)oxonium
(not *O*,*O*-dimethylcyclohexanecarboxylic acidium



$$\begin{array}{l}\overset{+}{N}(CH_3)_2\\ \|\\ CH_3-C\text{-}OH\end{array}$$

(1-hydroxyethylidene)di(methyl)azanium (PIN)
(1-hydroxyethylidene)di(methyl)ammonium
(not *N*,*N*-dimethylethanimidic acidium)

$$C_6H_5\text{-CO-}\overset{+}{S}(CH_3)_2$$

benzoyldi(methyl)sulfanium (PIN)
benzoyldi(methyl)sulfonium
(not *S*,*S*-dimethylbenzenecarbothioic acidium)

$$C_6H_5\text{-CO-O-}\overset{+}{O}H_2$$

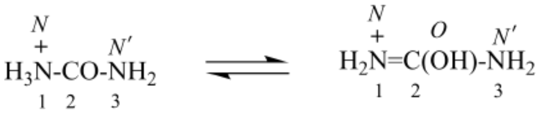
2-benzoyldioxidan-1-ium (PIN)
(not peroxybenzoic *OO*-acidium)

$$CH_3\text{-CO-}\overset{+}{Cl}\text{-}CH_3$$

acetyl(methyl)chloranium (PIN)

P-73.1.2.2 Uronium ions and chalcogen analogues

Cations derived formally by adding a hydron to urea (or isourea) are named on the basis of the parent cation ‘uronium’, representing the following tautomeric structures:



$$\underset{1}{\overset{N}{\overset{+}{H_3N}}}\text{-}\underset{2}{CO}\text{-}\underset{3}{\overset{N'}{NH_2}} \rightleftharpoons \underset{1}{\overset{N}{\overset{+}{H_2N}}}{=}\underset{2}{C}(\overset{O}{O}H)\text{-}\underset{3}{\overset{N'}{NH_2}}$$

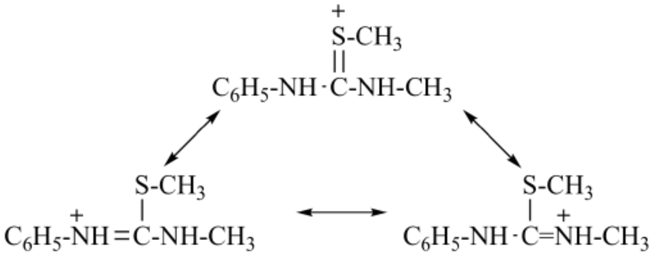
Numerical locants for the parent cation uronium are no longer used in preferred IUPAC names.

Locants follow those used for urea and isourea. Chalcogen analogues are named on the basis of parent cations, such as ‘thiouronium’, etc. This methodology leads to preferred IUPAC names.

Examples:

$$CH_3\text{-}\underset{3}{\overset{+}{N}H}{=}\underset{2}{C}(\text{-O-}C_6H_5)\text{-}\underset{1}{NH}\text{-}CH_3$$

N,*N*′-dimethyl-*O*-phenyluronium (PIN)
1,3-dimethyl-2-phenyluronium
N-[(methylamino)phenoxymethylidene]methanaminium



N,*S*-dimethyl-*N*′-phenylthiouronium (PIN)

P-73.2 CATIONIC COMPOUNDS WITH CATIONIC CENTERS DERIVED FORMALLY BY THE REMOVAL OF HYDRIDE IONS

P-73.2.1 Functional class names
P-73.2.2 Cationic centers in parent hydrides
P-73.2.3 Cationic centers on characteristic groups

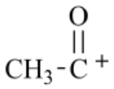
P-73.2.1 Functional class names

Cationic compounds that can be considered as being derived formally by removal of electrons from the corresponding radical may be named by adding the class name ‘cation’ as a separate word after the name of the radical. Polycations are indicated by adding the multiplying prefixes ‘di’, ‘tri’, etc., as appropriate, to the class name. Systematic names formed by using the suffix ‘ylium’ are preferred IUPAC names (see P-73.2.2). When the charge is not localized, the structure is enclosed in square brackets.

Examples:

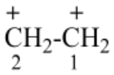
$^{+}CH_3$
methyl cation
methylium (PIN)

$[C_6H_5]^{+}$
phenyl cation
phenylium
benzenylium (PIN)



$CH_3\text{-}\overset{\overset{O}{\|}}{C}{}^{+}$

acetyl cation
acetylium (PIN)



$\underset{2}{\overset{+}{CH_2}}\text{-}\underset{1}{\overset{+}{CH_2}}$

ethane-1,2-diyl dication
ethane-1,2-bis(ylium) (PIN)

P-73.2.2 Cationic centers in parent hydrides

The following recommendations follow closely those for naming radicals, for which see P-71.

P-73.2.2.1 Cationic centers in parent hydrides
P-73.2.2.2 ‘Added indicated hydrogen’ for cations of mancude ring systems
P-73.2.2.3 Diazonium ions

P-73.2.2.1 Cationic centers in parent hydrides

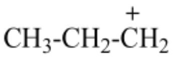
P-73.2.2.1.1 Specific method

Cations formed formally by the removal of a hydride ion, H^{-}, from a terminal atom of a saturated unbranched acyclic hydrocarbon, a saturated monocyclic hydrocarbon, or a mononuclear parent hydride belonging to Group 14, i.e., methane, CH_4, silane, SiH_4, germane, GeH_4, stannane, SnH_4, and plumbane, PbH_4, are named by replacing the ‘ane’ ending in the name of the parent hydride by the suffix ‘ylium’.

Examples:

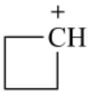
$^{+}CH_3$
methylium (PIN)

$(C_6H_5)_3Si^{+}$
triphenylsilylium (PIN)



$CH_3\text{-}CH_2\text{-}\overset{+}{CH_2}$

propylium (PIN)



cyclobutylium (PIN)

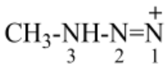
P-73.2.2.1.2 General method

According to the general method, cations formally derived by the removal of one hydride ion, H^{-}, from any position of a parent hydride are named by adding the suffix ‘-ylium’ to the name of the parent hydride, with elision of the final ‘e’ in the name of the parent hydride, if present. Di- and polycations formally derived by the removal of two or more hydride ions from the parent hydride are named by using the suffix ‘ylium’ and the multiplying prefixes ‘bis’, ‘tris’, etc. Preferred IUPAC names for the parent hydrides are used, as indicated in Chapters P-2 and P-5. In the examples that follow, preferred IUPAC names are indicated when traditional names are used in general nomenclature.

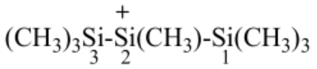
Examples:

H_2N^+
azanylium (preselected name)
aminylium
nitrenium

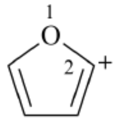
$C_6H_5\text{-}S^+$
phenylsulfanylium (PIN)

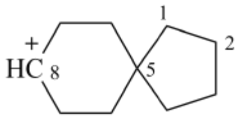

$CH_3\text{-}\underset{3}{N}H\text{-}\underset{2}{N}=\underset{1}{\overset{+}{N}}$

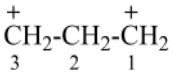
3-methyltriaz-1-en-1-ylium (PIN)


$(CH_3)_3\underset{3}{Si}\text{-}\underset{2}{\overset{+}{Si}}(CH_3)\text{-}\underset{1}{Si}(CH_3)_3$

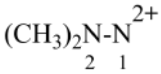
heptamethyltrisilan-2-ylium (PIN)


furan-2-ylium (PIN)

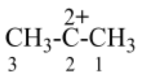

spiro[4.5]decan-8-ylium (PIN)


$\underset{3}{\overset{+}{C}}H_2\text{-}\underset{2}{C}H_2\text{-}\underset{1}{\overset{+}{C}}H_2$

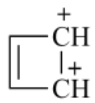
propane-1,3-bis(ylium) (PIN)

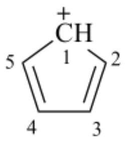

$(CH_3)_2\underset{2}{N}\text{-}\underset{1}{N}^{2+}$

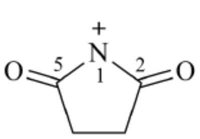
2,2-dimethylhydrazine-1,1-bis(ylium) (PIN)
2,2-dimethyldiazane-1,1-bis(ylium)


$\underset{3}{CH_3}\text{-}\underset{2}{\overset{2+}{C}}\text{-}\underset{1}{CH_3}$

propane-2,2-bis(ylium) (PIN)
1-methylethane-1,1-bis(ylium)


cyclobut-3-ene-1,2-bis(ylium) (PIN)

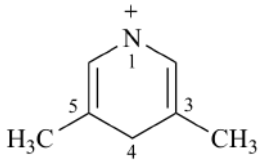

cyclopenta-2,4-dien-1-ylium (PIN)
cyclopentadienylium (see P-76)


2,5-dioxopyrrolidin-1-ylium (PIN)
succinimidylium

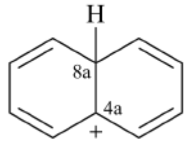
P-73.2.2.2 ‘Added indicated hydrogen’ for cations of mancude ring systems

A cationic center at a position in a mancude parent hydride where there is an insufficient number of hydrogen atoms to apply directly recommendations for the use of 'ylium' as given in P-73.2.2.1.2 is derived formally from a dihydro derivative of the cyclic parent hydride. Such a cation can also be described by applying the principle of 'added indicated hydrogen' (see P-14.7). In this method the 'hydro' derivative is described by specifying the hydrogen atom of a dihydro pair that remains after the cationic center is created by citing an italic capital H and the locant of the skeletal atom at which the hydrogen atom resides, both enclosed in a set of parentheses and inserted into the name of the corresponding parent hydride immediately after the locant for the cationic center. Names formed by the 'added indicated hydrogen' method are preferred IUPAC names (see P-58.2).

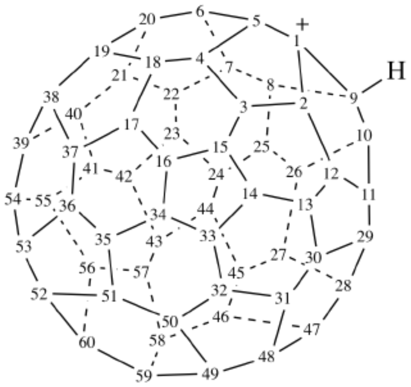
Examples:



3,5-dimethylpyridin-1(4*H*)-ylium (PIN)
3,5-dimethyl-1,4-dihydropyridin-1-ylium



naphthalen-4a(8a*H*)-ylium (PIN)
4a,8a-dihydronaphthalen-4a-ylium



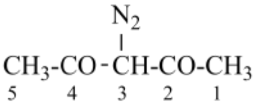
(C_{60}-*I*h)[5,6]fulleren-1(9*H*)-ylium (PIN)
1,9-dihydro(C_{60}-*I*h)[5,6]fulleren-1-ylium

P-73.2.2.3 Diazonium ions

Cations containing an $–N_2^+$ group attached to a parent hydride are traditionally named according to the principles of substitutive nomenclature by using the suffix 'diazonium' and the multiplying prefixes 'bis', 'tris', etc. to denote multiplicity. Diazonium ions may also be named on the basis of the parent cation 'diazenylium', $HN=N^+$. The use of the suffix 'diazonium' results in preferred IUPAC names.

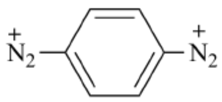
Examples:

$CH_3\text{-}N_2^+$
methanediazonium (PIN)
methyldiazenylium



$$\underset{5}{CH_3}\text{-}\underset{4}{CO}\text{-}\underset{3}{\overset{\overset{+}{N_2}}{CH}}\text{-}\underset{2}{CO}\text{-}\underset{1}{CH_3}$$

2,4-dioxopentane-3-diazonium (PIN)
(2,4-dioxopentan-3-yl)diazenylium



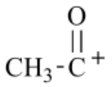
benzene-1,4-bis(diazonium) (PIN)
(1,4-phenylene)bis(diazenylium)

P-73.2.3 Cationic centers on characteristic groups

P-73.2.3.1 Acylium cations

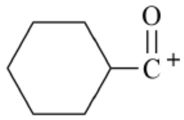
Cations formally derived by the removal of all the hydroxy groups as hydroxide ions from acids having systematic or retained names are named by replacing the ‘oic acid’ or ‘ic acid’ ending by the suffix ‘oylium’ or ‘ylium’, or the ‘carboxylic acid’ ending by ‘carbonylium’, in accordance with the rules for naming neutral acyl groups (see P-65.1.7). These names are preferred IUPAC names.

Examples:

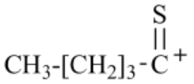


$CH_3\text{-}\overset{O}{\overset{\|}{C}}{}^{+}$

acetylium (PIN)
acetyl cation

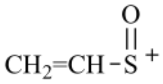


cyclohexanecarbonylium (PIN)
cyclohexanecarbonyl cation



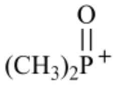
$CH_3\text{-}[CH_2]_3\text{-}\overset{S}{\overset{\|}{C}}{}^{+}$

pentanethioylium (PIN)



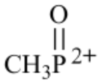
$CH_2{=}CH\text{-}\overset{O}{\overset{\|}{S}}{}^{+}$

ethenesulfinylium (PIN)



$(CH_3)_2\overset{O}{\overset{\|}{P}}{}^{+}$

dimethylphosphinoylium (PIN)



$CH_3\overset{O}{\overset{\|}{P}}{}^{2+}$

methylphosphonobis(ylium) (PIN)

P-73.2.3.2 Cations derived by the removal of a hydride ion from the nitrogen atom of an amide, amine, or imine characteristic group are named by using the appropriate suffixes for neutral groups modified by the addition of the suffix ‘ylium’, with elision of the final ‘e’ of the neutral suffix. Multiplying prefixes ‘bis-’, ‘tris-’, etc. are used to denote the multiplicity of these suffixes. Cations derived from imides are named on the basis of the appropriate heterocycle (see P-73.2.2.1.2). These names are the preferred IUPAC names; they are preferred to those formed by substitution of the appropriate parent cation.

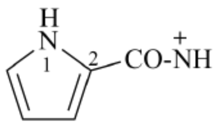
Examples:

$CH_3\text{-}CO\text{-}\overset{+}{N}H$

acetamidylium (PIN)

$CH_3\text{-}CH_2\text{-}\overset{+}{N}H$

ethanaminylium (PIN)



1*H*-pyrrole-2-carboxamidylium (PIN)

P-73.2.3.3 A cation derived formally by the removal of the hydrogen atom of a hydroxy group (or chalcogen analogue) of an acid or hydroxy characteristic group as a hydride ion is named as follows:

(1) additively, using the term ‘oxylium’ or ‘peroxylium’;

(2) by substituting the parent cations ‘oxidanylium’ or ‘dioxidanylium’ (preselected names) by the appropriate substituent groups.

The names methoxylium, ethoxylium, propoxylium, butoxylium and phenoxylium are retained as preferred IUPAC names, and aminoxylium as a preselected name. Otherwise, method (1) generates preferred IUPAC names.

Examples:

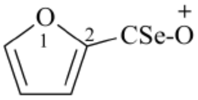
$CH_3\text{-}O^+$
methoxylium (PIN)
methyloxidanylium

$(CH_3)_3C\text{-}O\text{-}O^+$
tert-butylperoxylium (PIN)
tert-butyldioxidanylium

$Cl\text{-}CH_2\text{-}CO\text{-}O^+$
(chloroacetyl)oxylium (PIN)
chloroacetoxylium
(chloroacetyl)oxidanylium

$CH_3\text{-}CS\text{-}O^+$
(ethanethioyl)oxylium (PIN)
(ethanethioyl)oxidanylium

$(CH_3)_2N\text{-}O^+$
N-methylmethanaminoxylium (PIN)
(dimethylamino)oxidanylium



(furan-2-carboselenoyl)oxylium (PIN)
(furan-2-carboselenoyl)oxidanylium

P-73.2.3.4 Cationic centers on other characteristic groups

All other cationic centers are named by substituting the appropriate parent cation. In the case of sulfur cationic centers, the terms 'thioxylium' and 'dithioperoxylium', but not the term 'thioperoxylium' (ambiguity), may be used in general nomenclature. Use of the terms 'thiylium' or 'perthiylium' is not recommended.

Examples:

$Cl_2CH\text{-}CH_2\text{-}S^+$
(2,2-dichloroethyl)sulfanylium (PIN)
(2,2-dichloroethyl)thioxylium
[not 2,2-dichloro(ethylthiylium)]

$CH_3\text{-}CO\text{-}S^+$
acetylsulfanylium (PIN)
acetylthioxylium
(not acetylthiylium)

$C_6H_5\text{-}S\text{-}S^+$
phenyldisulfanylium (PIN)
phenyldithioperoxylium
(not phenylperthiylium)

$CH_3\text{-}CH_2\text{-}S\text{-}O^+$
(ethylsulfanyl)oxylium (PIN)
(ethylsulfanyl)oxidanylium
[not (ethylsulfanyl)thioperoxylium]

$CH_3\text{-}CH_2\text{-}N^{2+}$
ethylazanebis(ylium) (PIN)
[(not ethanaminebis(ylium)]

$C_6H_5\text{-}CO\text{-}N^{2+}$
benzoylazanebis(ylium) (PIN)
[not benzamidebis(ylium)]

$C_6H_5\text{-}CO\text{-}\underset{2}{N}H\text{-}\overset{+}{\underset{1}{N}}H$
2-benzoylhydrazin-1-ylium (PIN)

2-benzoyldiazan-1-ylium
(not benzohydrazid-*N*′-ium)

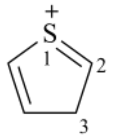
CH_3-CH_2-O-Te^+
ethoxytellanylium (PIN)
(not ethyltelluroperoxylium)

P-73.3 THE λ-CONVENTION WITH THE SUFFIX ‘YLIUM’

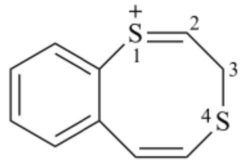
P-73.3.1 Application of the λ-convention with the suffix ‘ylium’

Cationic heterocycle having a cationic center on a heteroatom that has one more skeletal bonds than it has in the corresponding neutral heterocycle is named by adding the suffix ‘ylium’ to the name of the neutral parent hydride for which the λ-convention has been used to describe a nonstandard bonding state of the heteroatom, and that heteroatom has at least one hydrogen atom in the neutral heterocycle on which the ‘ylium’ suffix can operate. Indicated hydrogen (see P-14.7 and P-58.2.1) is used as needed.

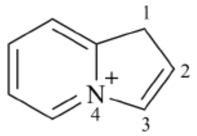
Examples:



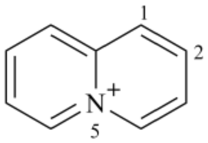
3*H*-1λ^4-thiophen-1-ylium (PIN)
(not 3*H*-thienylium)



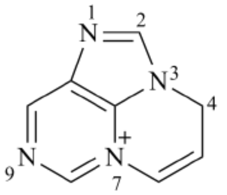
3*H*-1λ^4,4-benzodithiocin-1-ylium (PIN)



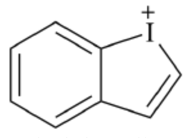
1*H*-4λ^5-indolizin-4-ylium (PIN)



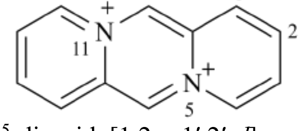
5λ^5-quinolizin-5-ylium (PIN)



4*H*-7λ^5-pyrimido[1,2,3-*cd*]purin-7-ylium (PIN)



1λ^3-benziodol-1-ylium (PIN)

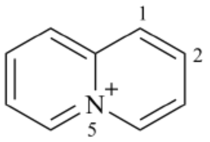


5λ^5,11λ^5-dipyrido[1,2-*a*:1′,2′-*d*]pyrazine-5,1

For certain cationic heterocycles of this type, especially those with cationic centers on heteroatoms from the second period elements, it might seem more acceptable to use replacement nomenclature (see P-73.4) or to derive the name by removal of two hydrogen atoms from a cation formed by addition of a hydron using the prefix ‘didehydro’, for example

‘4a-azonianaphthalene’ or ‘2,5-didehydro-2*H*-quinolizin-5-ium’ for the cation also known traditionally as quinolizinium.

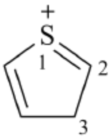
Example:



5λ^{5}-quinolizin-5-ylium (PIN)
4a-azonianaphthalene
(see P-73.4 for ‘azonia’)
2,5-didehydro-2*H*-quinolizin-5-ium

The ‘dehydro’ method, however, can become quite cumbersome, requiring both ‘hydro’ and ‘dehydro’ prefixes in some cases.

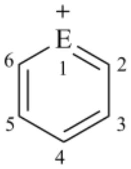
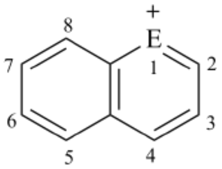
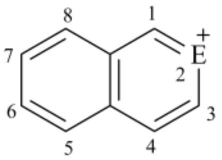
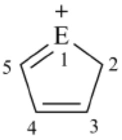
Example:

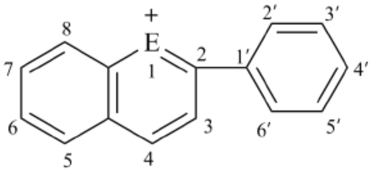


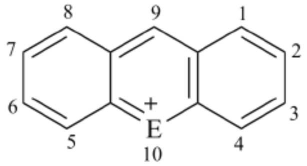
3*H*-1λ^{4}-thiophen-1-ylium (PIN)
1,2-didehydro-2,3-dihydrothiophen-1-ium
(not 3*H*-thienylium)

P-73.3.2 Retained names
The contracted and traditional names listed in Table 7.5 are retained as preferred IUPAC names and for use in general nomenclature.

Table 7.5 Retained names of ‘ylium’ cationic parent compounds

			
E = O	pyrylium (PIN)	E = O	1λ^{4}-benzopyran-1-ylium (PIN) chromenylium
E = S	thiopyrylium (PIN)	E = S	1λ^{4}-benzothiopyran-1-ylium (PIN) thiochromenylium
E = Se	selenopyrylium (PIN)	E = Se	1λ^{4}-benzoselenopyran-1-ylium (PIN) selenochromenylium
E = Te	telluropyrylium (PIN)	E = Te	1λ^{4}-benzotelluropyran-1-ylium (PIN) tellurochromenylium
		E = O	2λ^{4}-benzopyran-2-ylium (PIN) isochromenylium
		E = S	2λ^{4}-benzothiopyran-2-ylium (PIN) isothiochromenylium
		E = Se	2λ^{4}-benzoeselenopyran-2-ylium (PIN) isoselenochromenylium
		E = Te	2λ^{4}-benzotelluropyran-2-ylium (PIN) isotellurochromenylium
		E = O	2*H*-1λ^{4}-furan-1-ylium (PIN)
		E = S	2*H*-1λ^{4}-thiophen-1-ylium (PIN)
		E = Se	2*H*-1λ^{4}-selenophen-1-ylium (PIN)
		E = Te	2*H*-1λ^{4}-tellurophen-1-ylium (PIN)





E = O	flavylium	E = O	xanthylium (PIN)
E = S	thioflavylium	E = S	thioxanthylium (PIN)
E = Se	selenoflavylium	E = Se	selenoxanthylium (PIN)
E = Te	telluroflavylium	E = Te	telluroxanthylium (PIN)

P-73.4 SKELETAL REPLACEMENT (‘a’) NOMENCLATURE FOR CATIONS

Two methods are used to name cationic centers by skeletal replacement (‘a’) nomenclature:

(1) name the compound using neutral skeletal replacement (‘a’) prefixes and then describe the cationic centers by the appropriate suffix ‘ium’ and ‘ylium’;

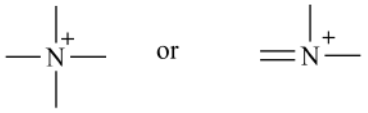
(2) by using cationic skeletal replacement (‘a’) prefixes.

Cationic skeletal replacement (‘a’) prefixes to indicate a cationic center having a bonding number one higher than the bonding number of the corresponding neutral mononuclear hydride, except for bismuth, are formed by replacing the ‘a’ ending of the normal skeletal replacement (‘a’) prefixes by ’onia’; the cationic skeletal replacement (‘a’) prefix corresponding to ‘bismuthonium’ is ‘bismuthonia’.

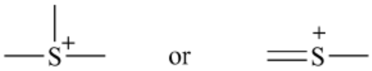
Cationic skeletal replacement (‘a’) prefixes to indicate a cationic center having a bonding number one lower than the bonding number of the corresponding neutral mononuclear hydride, except for carbon, are formed by replacing the final ‘e’ of the name of the fundamental parent hydride by ‘ylia’.

Cationic skeletal replacement (‘a’) prefixes are used in the same way as neutral replacement prefixes.

Examples:



azonia (preselected name)



thionia (preselected name)

$-\overset{+}{\mathrm{I}}-$

iodonia (preselected name)

$-\overset{+}{\mathrm{N}}-$

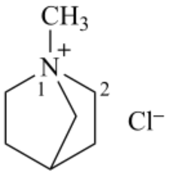
azanylia (preselected name)

$-\overset{+}{\mathrm{B}}-$

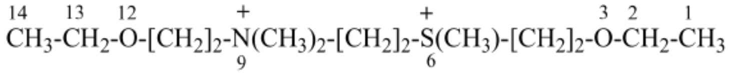
boranylia (preselected name)

Method (1) gives preferred IUPAC names. Furthermore, names that do not require designation of the skeletal atom in a nonstandard valence state by the λ-convention are preferred (see P-73.1 and P-73.2).

Examples:

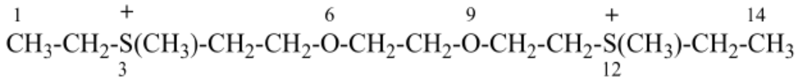


1-methyl-1-azabicyclo[2.2.1]heptan-1-ium chloride (PIN)
1-methyl-1-azoniabicyclo[2.2.1]heptane chloride



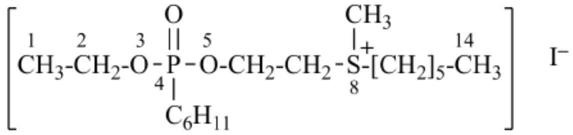
$\mathrm{CH_3\text{-}CH_2\text{-}O\text{-}[CH_2]_2\text{-}\overset{+}{N}(CH_3)_2\text{-}[CH_2]_2\text{-}\overset{+}{S}(CH_3)\text{-}[CH_2]_2\text{-}O\text{-}CH_2\text{-}CH_3}$

2-ethoxy-*N*-{2-[(2-ethoxyethyl)(methyl)sulfaniumyl]ethyl}-*N*,*N*-dimethylethanaminium (PIN)
{not 6,9,9-trimethyl-3,12-dioxa-6-thia-9-azatetradecane-6,9-diium;
nor 6,9,9-trimethyl-3,12-dioxa-6-thionia-9-azoniatetradecane;
the name must be based on a cation derived from the preferred amine name which is
2-ethoxy-*N*-{2-[(2-ethoxyethyl)(methyl)sulfanyl]ethyl}-*N*-methylethanamine and
not *N*-(2-ethoxyethyl)-2-[(2-ethoxyethyl)(methyl)sulfanyl]-*N*-methylethanamine
which is preferred alphanumerically, but does not qualify for a skeletal replacement ('a') name
because it does not have four heterounits}



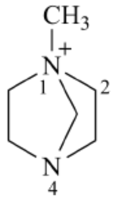
$\mathrm{CH_3\text{-}CH_2\text{-}\overset{+}{S}(CH_3)\text{-}CH_2\text{-}CH_2\text{-}O\text{-}CH_2\text{-}CH_2\text{-}O\text{-}CH_2\text{-}CH_2\text{-}\overset{+}{S}(CH_3)\text{-}CH_2\text{-}CH_3}$

3,12-dimethyl-6,9-dioxa-3,12-dithiatetradecane-3,12-diium (PIN)
3,12-dimethyl-6,9-dioxa-3,12-dithioniatetradecane

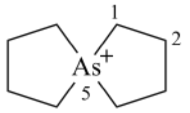


$\left[\mathrm{CH_3\text{-}CH_2\text{-}O\text{-}\underset{C_6H_{11}}{\overset{O}{\overset{\|}{P}}}\text{-}O\text{-}CH_2\text{-}CH_2\text{-}\overset{CH_3}{\overset{|}{\overset{+}{S}}}\text{-}[CH_2]_5\text{-}CH_3}\right]\ \mathrm{I^-}$

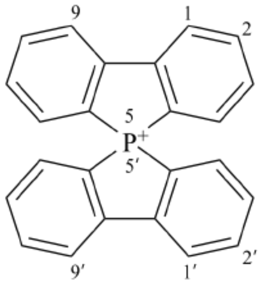
4-cyclohexyl-8-methyl-4-oxo-3,5-dioxa-8-thia-4λ^5-phosphatetradecan-8-ium iodide (PIN)
4-cyclohexyl-8-methyl-4-oxo-3,5-dioxa-8-thionia-4λ^5-phosphatetradecane iodide
(2-{[cyclohexyl(ethoxy)phosphinoyl]oxy}ethyl)hexyl(methyl)sulfonium iodide



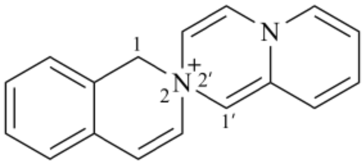
1-methyl-1,4-diazabicyclo[2.2.1]heptan-1-ium (PIN)



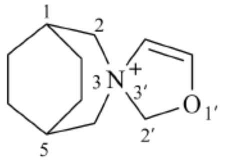
5λ^5-arsaspiro[4.4]nonan-5-ylium (PIN)
5-arsoniaspiro[4.4]nonane



5*H*-5λ^5,5′-spirobi[benzo[*b*]phosphindol]-5-ylium (PIN)
9-phosphonia-9,9′-spirobi[fluorene];
for construction of the name of the corresponding neutral, noncationic compound, see P-24.8.2)



1*H*-2λ^5-spiro[isoquinoline-2,2′-pyrido[1,2-*a*]pyrazin]-2-ylium (PIN)



2′*H*-3λ^5-spiro[3-azabicyclo[3.2.2]nonane-3,3′-[1,3]oxazol]-3-ylium (PIN)

P-73.5 CATIONIC COMPOUNDS WITH MULTIPLE CATIONIC CENTERS

Cationic compounds with multiple cationic centers are named by several methods in addition to previous rules.

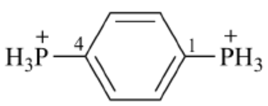
P-73.5.1 Assemblies of parent cations
P-73.5.2 'Ium' and 'ylium' centers in the same parent hydride
P-73.5.3 Cationic characteristic groups on parent cations

P-73.5.1 Assemblies of parent cations

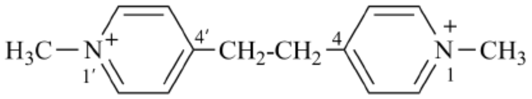
P-73.5.1.1 Assemblies derived from parent cations

Cationic compounds with cationic centers derived from the same parent hydride, but located in different parts of a structure, are named, if possible, according to the principles of multiplicative nomenclature (see P-15.3), using the multiplying prefixes 'bis-', 'tris-', etc. where necessary.

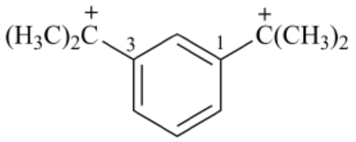
Examples:



(1,4-phenylene)bis(phosphanium) (PIN)
(1,4-phenylene)bis(phosphonium)



4,4′-(ethane-1,2-diyl)bis(1-methylpyridin-1-ium) (PIN)

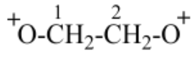


2,2′-(1,3-phenylene)di(propan-2-ylium) (PIN)

P-73.5.1.2 Polycations with cationic centers on characteristic groups

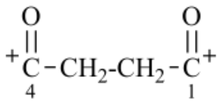
Polycations with cationic centers on characteristic groups are named by substitutive nomenclature or multiplicative nomenclature using the multiplying prefixes 'bis-', 'tris-', etc.

Examples:



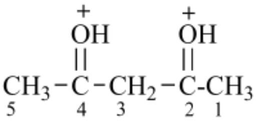
${}^{+}\text{O-}\overset{1}{\text{C}}\text{H}_2\text{-}\overset{2}{\text{C}}\text{H}_2\text{-O}^{+}$

(ethane-1,2-diyl)bis(oxylium) (PIN)
(ethane-1,2-diyl)bis(oxidanylium)



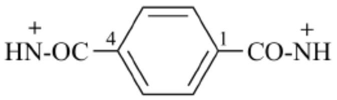
${}^{+}\underset{4}{\overset{\overset{\text{O}}{\|}}{\text{C}}}\text{-CH}_2\text{-CH}_2\text{-}\underset{1}{\overset{\overset{\text{O}}{\|}}{\text{C}}}{}^{+}$

1,4-dioxobutane-1,4-bis(ylium) (PIN)

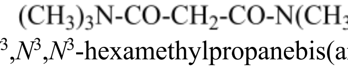


$\underset{5}{\text{CH}_3}\text{-}\underset{4}{\overset{\overset{+}{\text{O}}\text{H}}{\overset{\|}{\text{C}}}}\text{-}\underset{3}{\text{CH}_2}\text{-}\underset{2}{\overset{\overset{+}{\text{O}}\text{H}}{\overset{\|}{\text{C}}}}\text{-}\underset{1}{\text{CH}_3}$

(pentane-2,4-diylidene)bis(oxidanium) (PIN)
(pentane-2,4-diylidene)bis(oxonium)

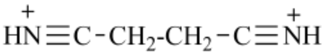


benzene-1,4-bis(carboxamidylium) (PIN)
(1,4-phenylenedicarbonyl)bis(azanylium)



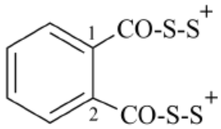
$(\text{CH}_3)_3\overset{+}{\text{N}}\text{-CO-CH}_2\text{-CO-}\overset{+}{\text{N}}(\text{CH}_3)_3$

N^1,N^1,N^1,N^3,N^3,N^3-hexamethylpropanebis(amidium) (PIN)
N,*N*,*N*,*N*′,*N*′,*N*′-hexamethylmalonamidium

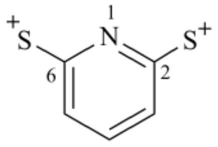


$H\overset{+}{N}{\equiv}C{-}CH_2{-}CH_2{-}C{\equiv}\overset{+}{N}H$

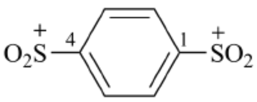
butanebis(nitrilium) (PIN)
butanediylidynebis(ammonium)
butanediylidynebis(azanium)



(benzene-1,2-dicarbonyl)bis(disulfanylium) (PIN)
(1,2-phenylenedicarbonyl)bis(disulfanylium)
(1,2-phenylenedicarbonyl)bis(dithioperoxylium)



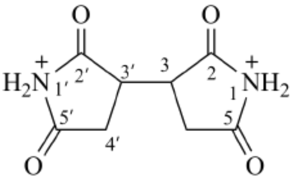
(pyridine-2,6-diyl)bis(sulfanylium) (PIN)
(pyridine-2,6-diyl)bis(thioxylium)



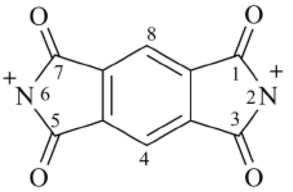
benzene-1,4-bis(sulfonylium)
(1,4-phenylene)bis(dioxo-λ^6-sulfanylium) (PIN)

P-73.5.1.3 Polycations derived from cyclic diimides and polyimides are named on the basis of the heterocyclic structure of the imides.

Examples:



2,2′,5,5′-tetraoxo[3,3′-bipyrrolidine]-1,1′-diium (PIN)



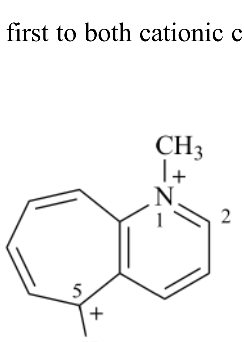
1,3,5,7-tetraoxo-5,7-dihydrobenzo[1,2-*c*:4,5-*c*′]dipyrrole-2,6(1*H*,3*H*)-bis(ylium) (PIN)

P-73.5.2 ‘Ium’ and ‘ylium’ centers in the same parent hydride

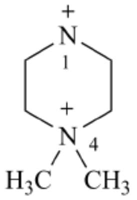
Cyclic compounds with two or more cationic centers in the same parent hydride structure at least one of which being denoted by ‘ium’ and another by ‘ylium’ suffixes, are named by placing the ‘ium’ and ‘ylium’ suffixes, in that order, after the name of the parent hydride, preceded by the appropriate multiplying numerical prefixes and locants, where required.

When there is a choice, low locants are assigned first to both cationic centers regardless of type (‘ium’ or ‘ylium’), and then to the ‘ylium’ centers.

Examples:



1-methyl-5*H*-cyclohepta[*b*]pyridin-1-ium-5-ylium (PIN)
[not 1-methyl-5*H*-1-azoniabenzo[7]annulen-5-ylium;
a skeletal replacement (‘a’) name is not recommended
when fusion names are possible (see P-25.5 and P-52.2.4.4)]

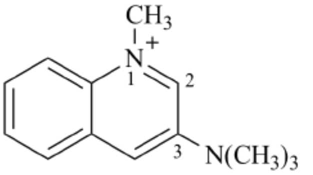


4,4-dimethylpiperazin-4-ium-1-ylium (PIN)

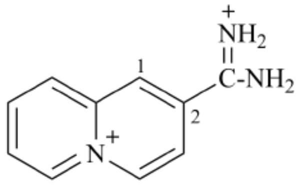
P-73.5.3 Cationic characteristic groups on parent cations

P-73.5.3.1 Cationic compounds with cationic centers both in the parent hydride part of the structure and on a characteristic group expressed as a cationic suffix are named by citing both cationic centers. The cationic center in the parent hydride is cited first followed by the cationic suffix.

Examples:



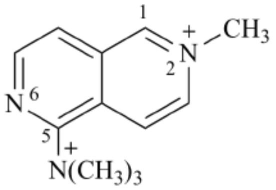
N,*N*,*N*,1-tetramethylquinolin-1-ium-3-aminium (PIN)



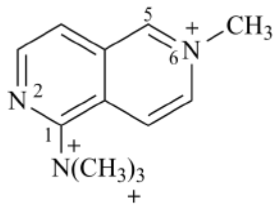
$5\lambda^5$-quinolizin-5-ylium-2-carboximidamidium (PIN)

P-73.5.3.2 Where there is a choice, low locants for skeletal cationic centers are determined before considering locants for cationic suffixes. This is consistent with the choice of lowest locants for corresponding neutral compounds (see P-14.4).

Example:



not



N,*N*,*N*,2-tetramethyl-2,6-naphthyridin-2-ium-5-aminium (PIN)
(not *N*,*N*,*N*,6-tetramethyl-2,6-naphthyridin-6-ium-1-aminium)

P-73.6 CATIONIC PREFIX NAMES

A polycation in which all cationic centers cannot be included in the cationic parent hydride or cationic parent compound is named by selecting one part of the structure as the parent cation and citing the other part(s) as cationic substituent prefixes. The selection of the parent cation is achieved by using the criteria for selecting the cationic parent structure. In zwitterions and in radical cations, the cationic part is always substituted into the anionic portion or into the part including a radical, in accordance with the seniority of anions and radicals over cations.

Two methods are used to name substituent structural units containing cationic centers:

(1) all prefix names are formed by adding the suffixes ‘yl’, ‘ylidene’, etc. to the cation name, preceded by the multiplying prefixes ‘di’, ‘tri’, etc. to indicate multiplicity and appropriate locants, where required. Where there is a choice for numbering, free valences receive lowest possible locants, the suffix ‘yl’ being senior to ‘ylidene’;

(2) prefixes for expressing a monovalent substituent derived from a mononuclear parent cation denoted by ‘ium’ or by ‘onium’ described in Table 7.3 are formed by changing the ‘onium’ ending of the parent cation to ‘io’ or ‘onio’.

Method (1) leads to preferred IUPAC names.

Examples:

$$-\overset{+}{\mathrm{N}}\mathrm{H}_3$$

azaniumyl (preselected prefix)
ammoniumyl
ammonio

$-\overset{+}{N}H_2\text{-}N{=}NH$

triaz-2-en-1-ium-1-yl (preselected prefix)
triaz-2-en-1-io

$-\underset{1}{\overset{+}{C}H_3}\text{-}\underset{2}{CH_3}$

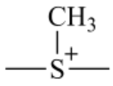
ethan-1-ium-1-yl (preferred prefix)

$-\underset{1}{CH_2}\text{-}\underset{2}{\overset{+}{C}}(CH_3)\text{-}\underset{3}{CH_3}$

2-methylpropan-2-ylium-1-yl (preferred prefix)

$-\overset{+}{Se}H_2$

selaniumyl (preselected prefix)
selenonio
selenoniumyl



$-\overset{CH_3}{\overset{|}{S^+}}-$

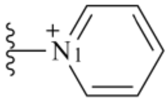
methylsulfaniumdiyl (preferred prefix)
methylsulfoniumdiyl

$-\overset{+}{N}\equiv N$

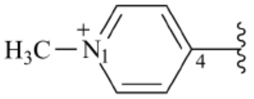
diazyn-1-ium-1-yl (preselected prefix)
diazonio

$=\overset{+}{N}(CH_3)_2$

N-methylmethanaminiumylidene (preferred prefix)
(not dimethylammoniumylidene)
(not dimethylimmonio)



pyridin-1-ium-1-yl (preferred prefix)
pyridinio



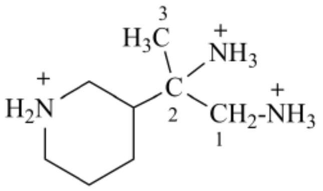
1-methylpyridin-1-ium-4-yl (preferred prefix)

P-73.7 CHOICE OF A PARENT STRUCTURE

A parent cationic structure is chosen by applying the following criteria in order until a definitive choice is achieved:

(a) parent with the maximum number of cationic, including cationic suffixes;

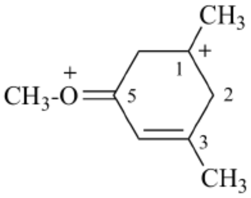
Example:



2-(piperidin-1-ium-3-yl)propane-1,2-bis(aminium) (PIN)
[not 3-(1,2-diaminiumylpropan-2-yl)piperidin-1-ium;
bis(aminium) is senior to piperidinium]

(b) parent with the maximum number of 'ylium' cationic centers with the exception of names based on the λ-convention (see P-73.8.2);

Example:



1,3-dimethyl-5-(methyloxidaniumylidene)cyclohex-3-en-1-ylium (PIN)
[not (1,5-dimethylcyclohex-4-en-1-ylium-3-ylidene)(methyl)oxidanium;
ylium is senior to ium]

(c) parent with the maximum number of senior cationic centers first cited in the seniority order of classes: N > P > As > Sb > Bi > Si > Ge > Sn > Pb > B > Al > Ga > In > Tl > O > S > Se > Te > C (see P-41);

> The seniority order for cations is now the order of seniority of classes rather than the order of skeletal replacement (‘a’) prefixes as used in RC-82.5.8.4, ref. 3.

Examples:

$$(\mathrm{CH_3})_3\overset{+}{\mathrm{P}}\text{-CH}_2\text{-[CH}_2]_4\text{-CH}_2\text{-}\overset{+}{\mathrm{S}}(\mathrm{CH_3})_2$$

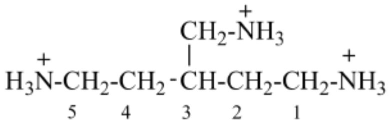
[6-(dimethylsulfaniumyl)hexyl]tri(methyl)phosphanium (PIN)
[not dimethyl[6-(trimethylphosphaniumyl)hexyl]sulfanium; P > S]

$$(\mathrm{CH_3})_3\overset{+}{\mathrm{N}}\text{-CH}_2\text{-[CH}_2]_4\text{-CH}_2\text{-}\overset{+}{\mathrm{S}}(\mathrm{CH_3})_2$$

6-(dimethylsulfaniumyl)-*N*,*N*,*N*-trimethylhexan-1-aminium (PIN)
{not dimethyl[6-(trimethylazaniumyl)hexyl]sulfanium; N> S}

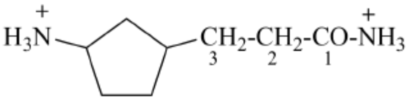
(d) further choice, if necessary, is made by applying the general criteria, giving priority to the corresponding suffixes (see Table 4.4) and by using the general seniority order of classes (see P-41) and parent structures (see P-44).

Examples:



$$\mathrm{H_3\overset{+}{N}\text{-}\underset{5}{CH_2}\text{-}\underset{4}{CH_2}\text{-}\underset{3}{\overset{\overset{CH_2\text{-}\overset{+}{N}H_3}{|}}{C}H}\text{-}\underset{2}{CH_2}\text{-}\underset{1}{CH_2}\text{-}\overset{+}{N}H_3}$$

3-(azaniumylmethyl)pentane-1,5-bis(aminium) (PIN)
(longest chain)



3-(3-azaniumylcyclopentyl)propanamidium (PIN)
(amidium is senior to aminium)

P-73.8 THE SUFFIXES ‘IUM’ vs. ‘YLIUM’ AND THE λ-CONVENTION

P-73.8.1 The suffix ‘-ylium’ is preferred to the suffix ‘-ium’ added to a parent hydride that has been modified by the λ-convention.

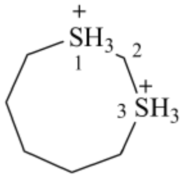
Example:

$\mathrm{H_2N^+}$
azanylium (preselected name)
λ^1-azanium
aminylium
nitrenium

P-73.8.2 The suffix ‘ium’ is preferred to the suffix ‘ylium’ added to a parent hydride that has been modified by the λ-convention; the suffix ‘ium’ is also preferred over ‘ylium’ when the λ-convention must be used to denote both cationic centers.

Examples:

$\mathrm{^+PH_4}$
phosphanium (preselected name)
phosphonium
λ^5-phosphanylium



1λ⁴,3λ⁴-dithiocane-1,3-diium (PIN)
1λ⁶,3λ⁶-dithiocane-1,3-bis(ylium)
(not 1λ⁶,3λ⁴-dithiocan-3-ium-1-ylium;
identical groups, if possible, must not be named differently within a name)

P-74 ZWITTERIONS

P-74.0 INTRODUCTION

Zwitterionic compounds have both positive and negative ionic centers. Most examples are essentially neutral because they have an equal number of formal unit charges of opposite sign and are best illustrated by the ionic forms of amino acids. The structures in this section are all represented as zwitterionic even though some can be drawn as neutral or ionic structures.

This section also includes inner salts and dipolar compounds. Section P-74.1 will cover zwitterionic compounds with the ionic centers on the same parent compound and with ionic centers on different parent structures. Section P-74.2 deals with 1,2- and 1,3-dipolar compounds.

According to the seniority of classes, an anionic center has priority over a cationic center in zwitterions. Thus, in zwitterionic compounds anionic centers are preferred for lower locants and become the parent structure, into which the cationic part is substituted. CAS gives cationic centers priority over anionic centers.

P-74.1 ZWITTERIONIC PARENT STRUCTURES HAVING THE ANIONIC AND CATIONIC CENTERS ON THE SAME PARENT COMPOUND INCLUDING IONIC CENTERS ON CHARACTERISTIC GROUPS EXPRESSIBLE AS SUFFIXES.

P-74.1.1 Ionic centers in the same parent structure

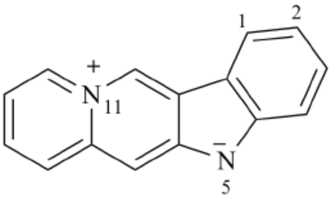
Zwitterionic compounds with the ionic centers in the same parent structure may be named by combining appropriate cumulative suffixes at the end of the name of a parent hydride in the order 'ium', 'ylium', 'ide', 'uide'. This method is preferred to the one using ionic replacement prefixes, as indicated in Sections P-72.4 and P-73.4. In either case anionic suffixes are cited after cationic suffixes in the name, and are given seniority for low locants. The final letter 'e' of the name of a parent hydride, or of an 'ide' or 'uide' suffix, is elided before the letter 'i' or 'y', or before a cumulative suffix beginning with a vowel. Multiplying prefixes 'di-', 'tri-', etc., or 'bis-', 'tris-', etc. as appropriate for each type of suffix, are added to specify the number of each kind of ionic center. Where there is a choice, lowest locants are given to the ionic centers in the following order, listed in decreasing order of seniority: 'uide' ('uida'), 'ide' ('ida'), 'ylium' ('ylia'), and 'ium' ('onia').

> For nomenclature purposes, zwitterionic compounds having the ionic centers in the same parent structure are not considered as neutral compounds. This is a change in the methodology described in RC-84.1.1 (ref. 3) and is illustrated in the last example below.

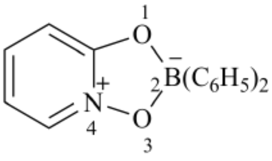
Examples:

$(CH_3)_3\overset{+}{N}\text{-}\overset{-}{N}\text{-}CH_3$

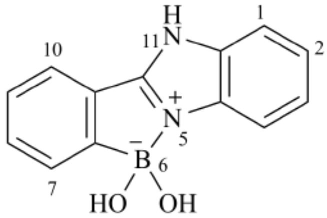
1,2,2,2-tetramethylhydrazin-2-ium-1-ide (PIN)



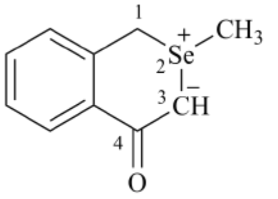
5*H*-11λ⁵-indolo[2,3-*b*]quinolizin-11-ylium-5-ide (PIN)



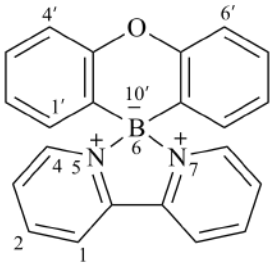
2,2-diphenyl-4λ⁵-[1,3,4,2]dioxazaborolo[4,5-*a*]pyridin-4-ylium-2-uide (PIN)



6,6-dihydroxy-6,11-dihydro-5λ^5-[1,3]benzimidazolo[1,2-*b*][2,1]benzazaborol-5-ylium-6-uide (PIN)
6,6-dihydroxy-6,11-dihydro-5λ^5-benzimidazolo[1,2-*b*][2,1]benzazaborol-5-ylium-6-uide



2-methyl-4-oxo-3,4-dihydro-1*H*-2-benzoselenopyran-2-ium-3-ide (PIN)
(not 2-methyl-3,4-dihydro-1*H*-2-benzoselenopyran-2-ium-3-id-4-one)
2-methyl-4-oxo-3,4-dihydro-1*H*-isoselenochromen-2-ium-3-ide
(not 2-methyl-3,4-dihydro-1*H*-isoselenochromen-2-ium-3-id-4-one)



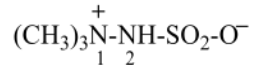
5λ^5,7λ^5-spiro[[1,3,2]diazaborolo[3,4-*a*:5,1-*a*′]dipyridine-6,10′-phenoxaborinine]-5,7-bis(ylium)-6-uide (PIN)

Note: For the name of this structure drawn as an intramolecular adduct, see P-68.1.6.2)

P-74.1.2 Zwitterionic compounds with at least one ionic center on a characteristic group

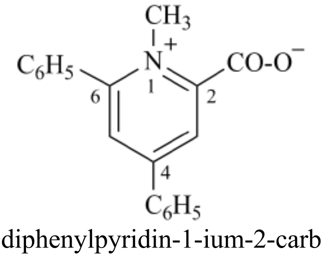
Zwitterionic compounds with at least one ionic center on a characteristic group may be named by adding the appropriate ionic suffix to the name of the ionic parent hydride. In names, cationic suffixes are cited before anionic suffixes. For assignment of lower locants, ionic centers on skeletal atoms of the parent hydride are preferred to the locants for positions of attachment of characteristic groups denoted by ionic suffixes.

Examples:

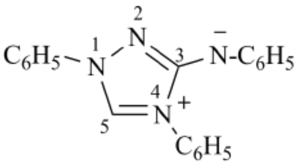


$(CH_3)_3\underset{1}{\overset{+}{N}}\text{-}\underset{2}{N}H\text{-}SO_2\text{-}O^-$

1,1,1-trimethylhydrazin-1-ium-2-sulfonate (PIN)



1-methyl-4,6-diphenylpyridin-1-ium-2-carboxylate (PIN)



N,1,4-triphenyl-1*H*-1,2,4-triazol-4-ium-3-aminide (PIN)
N-(1,4-diphenyl-1*H*-1,2,4-triazol-4-ium-3-yl)benzenaminide

P-74.1.3 Anionic and cationic centers on different parent structures

Zwitterionic compounds with anionic and cationic centers on different parent structures may be named by prefixing the name of the cationic center or the parts of the structure containing the cationic centers to the name of the anionic parent structure.

Examples:

$$(C_6H_5)_2\overset{+}{P}(CH_3)\text{-}CH{=}CH\text{-}\overset{-}{B}(CH_3)_3$$

trimethyl{2-[methyldi(phenyl)phosphaniumyl]ethen-1-yl}boranuide (PIN)
trimethyl{2-[methyldi(phenyl)phosphoniumyl]ethen-1-yl}boranuide

$$(CH_3)_3\overset{+}{N}\text{-}CH_2\text{-}CO\text{-}O^-$$

(*N*,*N*-dimethylmethanaminiumyl)acetate (PIN)
(trimethylammoniumyl)acetate

$$CH_3\text{-}\overset{-}{B}H_2\text{-}\underset{N'}{\overset{+}{N}}H_2\text{-}\overset{-}{B}H_2\text{-}\underset{N}{\overset{+}{N}}H_2\text{-}CH_3$$

methyl{[(methanaminiumyl)boranuidyl]azaniumyl}boranuide (PIN)
2,4-diaza-3,5-diborahexane-2,4-diium-
3,5-diuide 3,5-diazonia-2,4-diboranuidahexane
[not 1-methyl-3-(methanaminiumyl)diborazan-2-ium-1,3-diuide;
names such as diborazane are no longer named as parent hydrides, see P-21.2.3.1)

P-74.2 DIPOLAR COMPOUNDS

Dipolar compounds are electrically neutral molecules carrying a negative and a positive charge in at least one of their major canonical resonance structures. In most dipolar compounds the charges are delocalized; however the term is also applied to species where this is not the case. 1,2-Dipolar compounds have the opposite charges on adjacent atoms. The term 1,3-dipolar compounds is used for those in which a significant canonical resonance form can be represented by a separation of charge over three atoms.

P-74.2.1 1,2-Dipolar compounds
P-74.2.2 1,3-Dipolar compounds
P-74.2.3 Dipolar substituent groups

P-74.2.1 1,2-Dipolar compounds

P-74.2.1.1 ‘Ylides’

Compounds in which an anionic site ‘Y^-’ (originally only on carbon, but now including other atoms) is attached directly to a heteroatom ‘X^+’ (usually nitrogen, phosphorus, sulfur, selenium, or tellurium) carrying a formal positive charge are 1,2-dipolar species of the type $R_mX^+\text{-}Y^-\text{–}R_n$. If ‘X’ is a saturated atom of an element from the second row of the periodic system, the ‘ylide’ is commonly represented by a charge-separated form; if ‘X’ is a third, fourth, etc. row element uncharged canonical forms are usually shown, $R_mX{=}YR_n$.

These ‘ylides’ are subdivided into subclasses: nitrogen ylides, phosphorus ylides, oxygen ylides, sulfur ylides, etc. They may be named in different ways depending on the nature of the atoms ‘X’ and ‘Y’:

(1) as zwitterionic compounds;

(2) by applying the λ-convention when X = P, As, Sb, Bi, S, Se or Te;

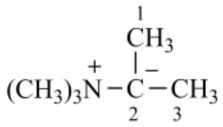
(3) by functional class nomenclature using the class names oxide, sulfide, imides.

Method (1) is applicable to all ‘ylides’ and leads to preferred IUPAC names.

P-74.2.1.1.1 Nitrogen ylides

Nitrogen ylides have the general structure $R_3N^+\text{–}C^-R_2$.

Example:



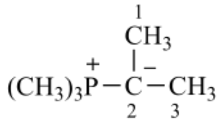
$$(CH_3)_3\overset{+}{N}-\underset{2}{\overset{\overset{1}{CH_3}\,|}{\overset{-}{C}}}-\underset{3}{CH_3}$$

(1) 2-(*N*,*N*-dimethylmethanaminiumyl)propan-2-ide (PIN)
2-(trimethylammoniumyl)propan-2-ide

P-74.2.1.1.2 Phosphorus ylides

Phosphorus ylides have the general structure $R_3P^+\text{–}C^-R_2 \leftrightarrow R_3P{=}CR_2$

Example:



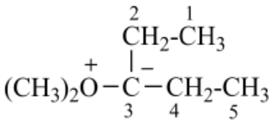
$$(CH_3)_3\overset{+}{P}-\underset{2}{\overset{\overset{1}{CH_3}}{\overset{|}{C}}}{}^{-}-\underset{3}{CH_3}$$

(1) 2-(trimethylphosphaniumyl)propan-2-ide (PIN)
2-(trimethylphosphoniumyl)propan-2-ide
(2) trimethyl(propan-2-ylidene)-λ^5-phosphane
(isopropylidene)tri(methyl)phosphorane

P-74.2.1.1.3 Oxygen ylides

Oxygen ylides have the general structure $R_2O^+–C^-R_2$.

Example:



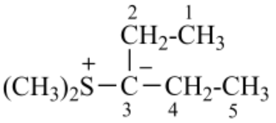
$$(CH_3)_2\overset{+}{O}-\underset{3}{\overset{\overset{2}{C}H_2\text{-}\overset{1}{C}H_3}{\overset{|}{C}}}{}^{-}-\underset{4}{CH_2}\text{-}\underset{5}{CH_3}$$

(1) 3-(dimethyloxidaniumyl)pentan-3-ide (PIN)
3-(dimethyloxoniumyl)pentan-3-ide

P-74.2.1.1.4 Sulfur ylides

Sulfur ylides have the general structure $R_2S^+–C^-R_2 \leftrightarrow R_2S{=}CR_2$.

Example:



$$(CH_3)_2\overset{+}{S}-\underset{3}{\overset{\overset{2}{C}H_2\text{-}\overset{1}{C}H_3}{\overset{|}{C}}}{}^{-}-\underset{4}{CH_2}\text{-}\underset{5}{CH_3}$$

(1) 3-(dimethylsulfaniumyl)pentan-3-ide (PIN)
3-(dimethylsulfoniumyl)pentan-3-ide
(2) dimethyl(pentan-3-ylidene)-λ^4-sulfane

This method is also applicable to the analogous selenium and tellurium compounds.

P-74.2.1.2 Amine oxides, imine oxides, and their chalcogen analogues

Amine oxides and imine oxides have the generic formulae $R_3N^+–O^-$ and $R_2C{=}N^+(R)–O^-$ respectively; chalcogen analogues are amine sulfides, imine selenides, etc. (where O is replaced by S, Se, or Te). They may be named:

(1) as zwitterionic compounds;

(2) by functional class nomenclature using the functional class name ‘oxide’, sulfide, ‘selenide’, or ‘telluride’.

Method (2) leads to preferred IUPAC names when one amine oxide is present. When two amine oxides are present, the λ-convention is used to generate PINs (see P-62.5). Hence, zwitterionic compounds are never PINs (see P-62.5).

Example:

$$(CH_3)_3\overset{+}{N}\text{-}O^-$$

(2) *N*,*N*-dimethylmethanamine *N*-oxide (PIN)
(trimethyl)amine oxide
(1) (trimethylazaniumyl)oxidanide
(trimethylammoniumyl)oxidanide

P-74.2.1.3 Amine imides

Amine imides (not amine imines) have the generic formula $R_3N^+–N^-–R$. They may be named by two methods:

(1) as a zwitterion based on hydrazine (in order not to break the nitrogen chain);

(2) by functional class nomenclature using the class name ‘imide’ placed after the name of the amine.

Method (1) leads to preferred IUPAC names.

Example:

$$(CH_3)_2\underset{2}{\overset{+}{N}}H\text{-}\underset{1}{\overset{-}{N}}\text{-}CH_3$$

(1) 1,2,2-trimethylhydrazin-2-ium-1-ide (PIN)
1,2,2-trimethyldiazan-2-ium-1-ide
(2) *N*-methylmethanamine *N*-methylimide
N,*N*′-dimethylmethanamine imide
(dimethyl)amine *N*-methylimide

P-74.2.1.4 Phosphine oxides and chalcogen analogues

Phosphine oxides have the generic formula $R_3P^+–O^-$ ↔ $R_3P{=}O$. Chalcogen analogues are phosphine sulfides, phosphine selenides, and phosphine telluride (where O is replaced by S, Se, and Te, respectively). They may be named by three methods:

(1) as zwitterionic compounds;

(2) by functional class nomenclature using the class names oxide, sulfide, selenide, or telluride;

(3) substitutively, as heterones, by using the suffix ‘-one’ and λ^5-phosphane as the parent hydride.

Method (3) leads to preferred IUPAC names.

Example:

$$(C_6H_5)_3\overset{+}{P}\text{-}\overset{-}{O}$$

(3) triphenyl-λ^5-phosphanone (PIN)
(2) triphenylphosphane oxide
(1) (triphenylphosphaniumyl)oxidanide
(triphenylphosphoniumyl)oxidanide

These methods are also applied to arsine and stibine oxides, sulfides, etc.

P-74.2.1.5 Phosphine imides

Phosphine imides have the generic structure: $R_3P^+–N^-–R$ ↔ $R_3P{=}N–R$. They may be named in three ways:

(1) as zwitterionic compounds;

(2) by functional class nomenclature using the class name imide;

(3) substitutively, as heterimines, by using the suffix ‘-imine’ and λ^5-phosphane as the parent hydride.

Method (3) leads to preferred IUPAC names.

Example:

$$(C_6H_5)_3\overset{+}{P}\text{-}\overset{-}{N}\text{-}CH_2\text{-}CH_3$$

(3) *N*-ethyl-*P*,*P*,*P*-triphenyl-λ^5-phosphanimine (PIN)
(1) ethyl(triphenylphosphaniumyl)azanide
(2) triphenylphosphane *N*-ethylimide
N-ethyl-*P*,*P*,*P*-triphenylphosphane imide
N-ethyl-*P*,*P*,*P*-triphenylphosphine imide

These methods are also applied to arsine and stibine imides.

P-74.2.2 1,3-Dipolar compounds

The term 1,3-dipolar compounds is used for those compounds in which a significant canonical resonance can be represented by a distribution of charge over three atoms. The subclasses of 1,3-dipolar compounds include:

P-74.2.2.1 the allyl (propenyl) type
P-74.2.2.2 the propargyl (prop-2-yn-1-yl) type
P-74.2.2.3 the carbene type

P-74.2.2.1 Allyl type compounds have the following delocalized general structure where Y and/or Z = C, N, or O; and X = N or O:

$$Z{=}X^+\text{-}Y^- \leftrightarrow Z^-\text{-}X^+{=}Y \leftrightarrow Z^+\text{-}X\text{-}Y^- \leftrightarrow Z^-\text{-}X\text{-}Y^+$$

Preferred IUPAC names are based on the first canonical form, although each canonical form can be named, if so desired. Names are formed in four different ways:

(1) by using a parent hydride to generate a zwitterion;

(2) by substituting a cationic substituent into a parent anion;

(3) by functional class nomenclature using the class names imide, oxide, etc.;

(4) by using the λ-convention.

Preferred IUPAC names are those expressing the zwitterionic nature of the compounds. Three exceptions are recognized:

(1) heteroatom oxides as described in P-74.2.2.1.4 for azoxy compounds and as described in P-74.2.2.1.9 for nitrones;

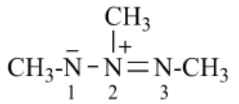
(2) use of the λ-convention as in P-74.2.2.1.8 for heterone *S*-oxides.

P-74.2.2.1.1 Azo imides, analogous to azoxy compounds, have the following delocalized general structure:

$$RN{=}N^+(R){-}N^-{-}R{-} \quad \leftrightarrow \quad RN^-{-}N^+(R){=}NR$$

Method (1) in P-74.2.2.1 gives preferred IUPAC names.

Example:



$$CH_3\text{-}\underset{1}{\bar{N}}\text{-}\underset{2}{\overset{CH_3}{\overset{|+}{N}}}{=}\underset{3}{N}\text{-}CH_3$$

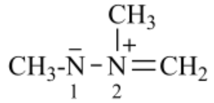
1,2,3-trimethyltriaz-2-en-2-ium-1-ide (PIN;
the preferred name is based on the unbroken nitrogen chain)
dimethyldiazene methylimide
trimethyldiazene imide
[methyl(methylimino)ammoniumyl]methanaminide

P-74.2.2.1.2 Azomethine imides have the following delocalized general structure:

$$R\text{-}N^-{-}N^+(R){=}CR_2 \quad \leftrightarrow \quad R\text{-}N{=}N^+(R)\text{-}C^-R_2$$

Method (1) in P-74.2.2.1 gives preferred IUPAC names.

Example:



$$CH_3\text{-}\underset{1}{\bar{N}}\text{-}\underset{2}{\overset{CH_3}{\overset{|+}{N}}}{=}CH_2$$

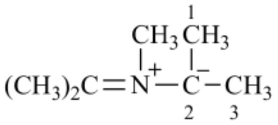
1,2-dimethyl-2-methylidenehydrazin-2-ium-1-ide (PIN)
N-methylmethanimine methylimide

P-74.2.2.1.3 Azomethine ylides have the following delocalized general structure:

$$R_2C^-{-}N^+(R){=}CR_2 \quad \leftrightarrow \quad R_2C{=}N^+(R)\text{-}C^-R_2$$

Method (2) in P-74.2.2.1 gives preferred IUPAC names.

Example:

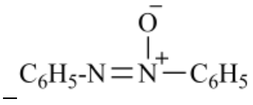


$$(CH_3)_2C{=}\overset{CH_3}{\overset{|+}{N}}{-}\underset{2}{\overset{\overset{1}{CH_3}}{\overset{|-}{C}}}{-}\underset{3}{CH_3}$$

2-(*N*-methylpropan-2-iminiumyl)propan-2-ide (PIN)
2-[methyl(propan-2-ylidene)ammoniumyl]propan-2-ide

P-74.2.2.1.4 Azoxy compounds have the general structure $R\text{-}N{=}N^+(O^-)\text{-}R$ (see also P-68.3.1.3.3.1). Method (3) in P-74.2.2.1 gives preferred IUPAC names.

Example:



$\mathrm{C_6H_5\text{-}N{=}\overset{\overset{\bar{O}}{|}}{N^{+}}{-}C_6H_5}$

diphenyldiazene oxide (PIN)
(diphenyldiazeniumyl)oxidanide
azoxybenzene
1,2-diphenyl-1λ^5-diazen-1-one

P-74.2.2.1.5 Carbonyl imides have the following delocalized general structure:

$$R_2C{=}O^+{-}N^-\text{-}R \quad \leftrightarrow \quad R_2C^+{-}O\text{-}N^-\text{-}R$$

Method (2) in P-74.2.2.1 gives preferred IUPAC names.

Example:

$$\mathrm{(CH_3)_2C{=}\overset{+}{O}\text{-}\bar{N}\text{-}CH_3}$$

N-[(propan-2-ylidene)oxidaniumyl]methanaminide (PIN)
N-[(propan-2-ylidene)oxoniumyl]methanaminide
propan-2-one methylimide
N-methylpropan-2-one imide

P-74.2.2.1.6 Carbonyl oxides have the following delocalized general structure:

$$R_2C^-{-}O^+{=}O \quad \leftrightarrow \quad R_2C{=}O^+\text{-}O^-$$

Method (1) in P-74.2.2.1 gives preferred IUPAC names.

Example:

$$\mathrm{(CH_3)_2C{=}\overset{+}{O}{-}\bar{O}}$$

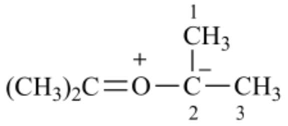
2-(propan-2-ylidene)dioxidan-2-ium-1-ide (PIN)
propan-2-one oxide

P-74.2.2.1.7 Carbonyl ylides have the following delocalized general structure:

$$R_2C{=}O^+{-}C^-(R)_2 \quad \leftrightarrow \quad R_2C^+{-}OC^-(R)_2$$

Method (2) in P-74.2.2.1 gives preferred IUPAC names.

Example:



$\mathrm{(CH_3)_2C{=}\overset{+}{O}{-}\underset{2}{\overset{\overset{\overset{1}{CH_3}}{|}}{C^-}}{-}\underset{3}{CH_3}}$

2-[(propan-2-ylidene)oxidaniumyl]propan-2-ide (PIN)
2-[(propan-2-ylidene)oxoniumyl]propan-2-ide

P-74.2.2.1.8 Thioaldehyde *S*-oxides, thioketone *S*-oxides, and heterone *S*-oxides have the following delocalized general structure:

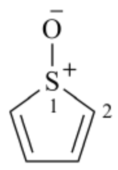
$$RR'C{=}S^+{-}O^- \quad \leftrightarrow \quad RR'C{=}S{=}O \text{ (where } R' = \text{ or } \neq H)$$

Method (4) in P-74.2.2.1 gives preferred IUPAC names.

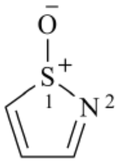
Examples:

$$\mathrm{CH_3\text{-}CH_2\text{-}CH{=}\overset{+}{S}{-}\bar{O}}$$

propylidene-λ^4-sulfanone (PIN)
propanethial oxide
(propylidenesulfaniumyl)oxidanide
1-(oxo-λ^4-sulfanylidene)propane



1*H*-1λ^4-thiophen-1-one (PIN)
thiophene oxide
(thiophen-1-ium-1-yl)oxidanide
1-oxo-1*H*-1λ^4-thiophene



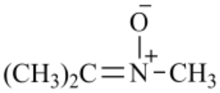
1*H*-1λ⁴,2-thiazol-1-one (PIN)
1,2-thiazole 1-oxide
1,2-thiazole *S*-oxide

P-74.2.2.1.9 Nitrones have the following delocalized general structure:

$R_2C{=}N^+(O^-)R'$ ↔ $R_2C^+{-}N(O^-)R'$ where $R' \neq H$; compounds where $R' = H$ are not included in this class

Method (3) in P-74.2.2.1 gives preferred IUPAC names.

Example:

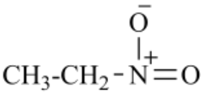


$$(CH_3)_2C{=}\overset{\overset{\displaystyle \bar{O}}{|}}{N^+}{-}CH_3$$

N-methylpropan-2-imine *N*-oxide (PIN)
[methyl(propan-2-ylidene)azaniumyl]oxidanide

P-74.2.2.1.10 Nitro compounds are named on the basis of the traditional structure, $R{-}NO_2$, using the compulsory prefix ‘nitro’ (see also P-61.5.1).

Example:



$$CH_3{-}CH_2{-}\overset{\overset{\displaystyle \bar{O}}{|}}{N^+}{=}O \leftrightarrow CH_3{-}CH_2{-}NO_2$$

nitroethane (PIN)

P-74.2.2.2 The propargyl (propynyl) type includes compounds having the following canonical resonance forms:

$X{\equiv}N^+{-}Z^-$ ↔ $^-X{=}N^+{=}Z$ ↔ $^-X{=}N{-}Z^+$,
where X = C, N or O; and Z = C, N or O

P-74.2.2.2.1 Nitrile imides, nitrile oxides and chalcogen analogues, and nitrile ylides may be named in two different ways:

(1) as zwitterionic compounds, without breaking the longest chain of heteroatoms;

(2) by functional class nomenclature using the class names imide, oxide, sulfide, etc.

P-74.2.2.2.1.1 Nitrile imides.

Method (1) in P-74.2.2.2.1, zwitterionic names, generates preferred IUPAC names.

Example:

$$CH_3{-}C{\equiv}\underset{2}{\overset{+}{N}}{-}\underset{1}{\overset{-}{N}}{-}CH_3$$

2-ethylidyne-1-methylhydrazin-2-ium-1-ide (PIN)
acetonitrile methylimide

P-74.2.2.2.1.2 Nitrile oxides and chalcogen analogues.

Method (2) in P-74.2.2.2.1, functional class names, yields preferred IUPAC names (see also P-66.5.4.1).

Examples:

$$CH_3{-}C{\equiv}\overset{+}{N}{-}\bar{O}$$

acetonitrile oxide (PIN)
(ethylidyneazaniumyl)oxidanide

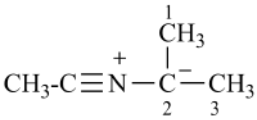
$$CH_3{-}C{\equiv}\overset{+}{N}{-}\bar{S}$$

acetonitrile sulfide (PIN)
(ethylidyneazaniumyl)sulfanide

P-74.2.2.2.1.3 Nitrile ylides

Method (1) in P-74.2.2.2.1, zwitterionic names, gives preferred IUPAC names.

Example:



$$\mathrm{CH_3{-}C{\equiv}\overset{+}{N}{-}\overset{\overset{1}{CH_3}}{\underset{2}{C^{-}}}{-}\underset{3}{CH_3}}$$

2-(acetonitriliumyl)propan-2-ide (PIN)
2-(ethylidyneammoniumyl)propan-2-ide

P-74.2.2.2.2 Azides may be named by three methods:

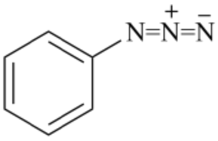
(1) substitutively, using the compulsory prefix azido (P-61.7);

(2) by functional class nomenclature using the class name azide;

(3) as derivatives of the zwitterionic parent hydride ‘triazadien-2-ium-1-ide.’

Method (1) yields preferred IUPAC names (see also P-61.7)

Example:



azidobenzene (PIN)
phenyl azide
3-phenyltriazadien-2-ium-1-ide

P-74.2.2.2.3 Diazo compounds may be named in two ways:

(1) substitutively by using the compulsory prefix diazo (P-61.4);.

(2) as derivatives of the zwitterionic parent hydride diazen-2-ium-1-ide.

Method (1) leads to preferred IUPAC names (see also P-61.4).

Example:

$$\mathrm{H_2C{=}\overset{+}{N}{=}\overset{-}{N}}$$

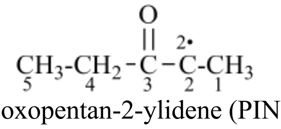
diazomethane (PIN)
methylidenediazen-2-ium-1-ide

P-74.2.2.3 The carbene type includes compounds having the following canonical resonance forms:

$X^{2\bullet}\text{-}C{=}Z \leftrightarrow {}^{+}X{=}C\text{-}Z^{-}$,
where X = C or N and Z = C, N or O

P-74.2.2.3.1 Acyl carbenes have the generic structure acyl-$C^{2\bullet}$–R. In organic chemistry, an unspecified acyl carbene is generally a carbonyl carbene and may be named by using the longest carbon chain, according to the principles of substitutive nomenclature for radicals (see P-71.2), priority being given to the radical to be cited as the suffix

Example:



$$\mathrm{\underset{5}{CH_3}{-}\underset{4}{CH_2}{-}\underset{3}{\overset{\overset{O}{||}}{C}}{-}\underset{2}{\overset{2\bullet}{C}}{-}\underset{1}{CH_3}}$$

3-oxopentan-2-ylidene (PIN)

P-74.2.2.3.2 Imidoyl carbenes

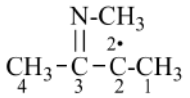
Compounds having the structure RC(=NH)-$C^{2\bullet}$–R are imidoyl carbenes. Imidoyl is a shortened, but imprecise, term for carboximidoyl, RC(=NH)–. These carbenes may be named by two methods:

(1) by using the longest carbon chain, according to the principles of substitutive nomenclature for radicals, low locants being assigned to the radical to be cited as suffix;

(2) substitutively on the basis of the appropriate carbene as the parent structure.

Method (1) leads to preferred IUPAC names.

Example:



$$\underset{4}{CH_3}\text{-}\underset{3}{\overset{\overset{\text{N-CH}_3}{||}}{C}}\text{-}\underset{2}{\overset{2\bullet}{C}}\text{-}\underset{1}{CH_3}$$

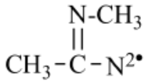
3-(methylimino)butan-2-ylidene (PIN)

P-74.2.2.3.3 Imidoyl nitrenes have the following general structure:

$$RC(=N\text{-}R')N^{2\bullet} \leftrightarrow RC(N^{-}\text{-}R')=N^{+}$$

They may be named substitutively using the parent names azanylidene, nitrene, or aminylene. The use of ‘azanylidene’ leads to preferred IUPAC names.

Example:



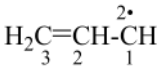
$$CH_3\text{-}\overset{\overset{\text{N-CH}_3}{||}}{C}\text{-}N^{2\bullet}$$

(*N*-methylethanimidoyl)azanylidene (PIN)
(*N*-methylacetimidoyl)nitrene
(*N*-methylacetimidoyl)aminylene

P-74.2.2.3.4 Vinyl (ethenyl) carbenes have the structure RR′C=CR″-$C^{2\bullet}$-R‴.

Preferred IUPAC names are formed by using the longest carbon chain according to the principles of substitutive nomenclature for radicals, low locants being assigned to the suffix ‘ylidene’.

Example:



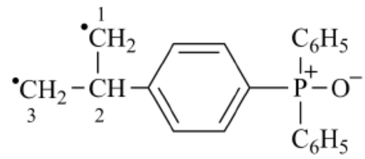
$$\underset{3}{H_2C}=\underset{2}{CH}\text{-}\underset{1}{\overset{2\bullet}{CH}}$$

prop-2-en-1-ylidene (PIN)

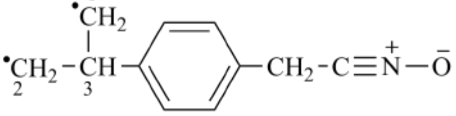
P-74.2.3 Dipolar substituent groups

Names of dipolar substituent groups are formed by using prefixes for naming ions as the substituent group and designating the free valences by the suffixes ‘yl’, ‘ylidene’ or ‘ylidyne’.

Examples:



2-{4-[oxidodi(phenyl)phosphaniumyl]phenyl}propane-1,3-diyl (PIN)
2-{4-[oxidodi(phenyl)phosphoniumyl]phenyl}propane-1,3-diyl



2-{4-[2-(oxidoazaniumylidyne)ethyl]phenyl}propane-1,3-diyl (PIN)
2-{4-[2-(oxidoammoniumylidyne)ethyl]phenyl}propane-1,3-diyl

P-75 RADICAL IONS

For the purpose of nomenclature of organic chemistry, a radical ion is a molecular entity having at least one radical center and one ionic center, which may be on the same or on different atoms of a parent structure. They are formally named as described in the following subsections.

P-75.1 Radical ions formed by the addition or removal of electrons
P-75.2 Radical ions derived from parent hydrides
P-75.3 Radical ions on characteristic groups
P-75.4 Ionic and radical centers in different parent structures

P-75.1 RADICAL IONS FORMED BY THE ADDITION OR REMOVAL OF ELECTRONS

Radical ions formed by the addition or removal of electrons may be named in two ways.

(1) by using the suffixes ‘elide’ and ‘elium’ in substitutive nomenclature, whereby radical ions derived formally from a neutral parent hydride, parent compound, or hydro derivative of either by the addition or removal of

electrons may be named by adding the suffixes ‘elide’ or ‘elium’ to the name of the neutral parent structure, the number of added or removed electrons is denoted by numerical prefixes, ‘di’, ‘tri’, etc.

Note: This new method may be used to indicate a global structure, when the positions of the radical and/or ionic centers are not known, or when it is not necessary, nor desirable, to name a specific structure. These suffixes cannot be used in the presence of other suffixes.

(2) by functional class nomenclature, whereby radical ions derived formally from a neutral parent hydride, parent compound, or hydro derivative of either by the addition or removal of electrons may be named by adding the terms ‘radical cation’ or ‘radical anion’ as separate words to the name of the neutral parent hydride or parent compound having the same molecular formula; the multiplying prefixes ‘di’, ‘tri’ etc. are used to denote multiple radical or ionic centers; the terms ‘radical ion’ can also be used, followed by a charge number indicating the appropriate charge sign.

The substitutive method (1) leads to preferred IUPAC names.

Examples:

$[C_6H_5\text{-}C_6H_5]^{(2\bullet)(2-)}$
[1,1′-biphenyl]dielide (PIN)
biphenyl diradical dianion
biphenyl diradical ion(2–)

$[C_{10}H_8]^{\bullet+}$
azulenelium (PIN)
azulene radical cation
azulene radical ion(1+)

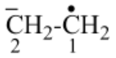
P-75.2 RADICAL IONS DERIVED FROM PARENT HYDRIDES

The order of seniority, radicals > anions > cations, is reflected in a preferred IUPAC name. Suffixes assigned to anionic and/or cationic centers are placed first after the name of the parent structure (parent hydride, functional parent hydride, or functionalized parent hydride), followed by suffixes attributed to radical centers.

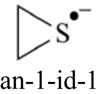
A radical ion derived formally by the removal of one or more hydrogen atoms from a single skeleton atom or from different skeletal atoms of an ionic or zwitterionic parent hydride is named by adding to its name the suffixes ‘yl’ or ‘ylidene’ with appropriate multiplying prefixes before ‘yl’ or ‘ylidene’, with elision of the final letter ‘e’ of the name of the ionic parent hydride. Skeletal positions with radical centers have preference over those with ionic centers for assignment of low locants.

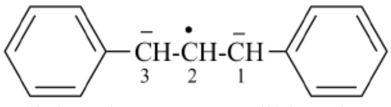
P-75.2.1 Examples of radical anions:

$HN^{\bullet-}$
azanidyl (preselected name)
aminidyl


$\underset{2}{\overset{-}{C}H_2}\text{-}\underset{1}{\overset{\bullet}{C}H_2}$
ethan-2-id-1-yl (PIN)

$(CH_3)_3B^{\bullet-}$
trimethylboranuidyl (PIN)
trimethyl-1λ^5-boranidyl


1λ^4-thiiran-1-id-1-yl (PIN)


1,3-diphenylpropane-1,3-diid-2-yl (PIN)

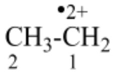
$CH_3\text{-}O\text{-}CO\text{-}C^{2\bullet-}$
(methoxycarbonyl)methanidylidene (PIN)

P-75.2.2 Examples of radical cations:

$H_2C^{\bullet+}$
methyliumyl (PIN)

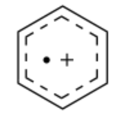
$H_4Si^{\bullet+}$
silaniumyl (preselected name)

$[CH_3\text{-}CH_2]^{\bullet 2+}$
ethaniumyliumyl (PIN)
(location of radical and ionic centers is unknown)



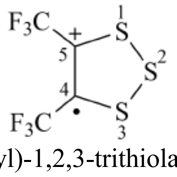
$$\underset{2}{CH_3}\text{-}\overset{\bullet 2+}{\underset{1}{CH_2}}$$

ethan-1-ium-1-ylium-1-yl (PIN)
(location of radical and ionic centers as indicated by locants)



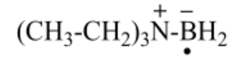
or $[C_6H_6]^{\bullet+}$

benzenelium (PIN)
benzeniumyl



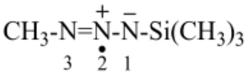
4,5-bis(trifluoromethyl)-1,2,3-trithiolan-5-ylium-4-yl (PIN)

P-75.2.3 Examples of zwitterionic radical ions:



$$(CH_3\text{-}CH_2)_3\overset{+}{N}\text{-}\underset{\bullet}{\overset{-}{B}}H_2$$

(*N*,*N*-diethylethanaminiumyl)boranuidyl (PIN)



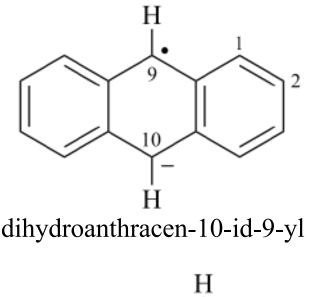
$$CH_3\text{-}\underset{3}{N}=\underset{\underset{2}{\bullet}}{\overset{+}{N}}\text{-}\underset{1}{\overset{-}{N}}\text{-}Si(CH_3)_3$$

3-methyl-1-(trimethylsilyl)triaz-2-en-2-ium-1-id-2-yl (PIN)

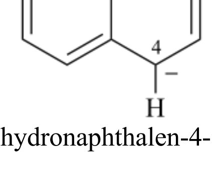
P-75.2.4 ‘Added indicated hydrogen’

Radical and ionic centers at positions in a mancude parent hydride where there is an insufficient number of hydrogen atoms to directly apply recommendations for the use of ‘yl’, ‘ylidene’, ‘ide’ or ‘ylium’ as given in P-71.1, P-72.1 and P-73.2, respectively are derived formally from a dihydro derivative of the cyclic parent hydride. Radical ions can also be described by applying the principle of ‘added indicated hydrogen’ (see P-14.7 and P-58.2.2). In this method, the ‘hydro’ derivative is described by specifying the hydrogen atom of a dihydro pair that remains after the radical center is created by citing in italic capital H and the locant of the skeletal atom to which the hydrogen atom resides, both enclosed in a set of parentheses and inserted into the name of the corresponding parent hydride immediately after the locant for the radical center. The ionic center is created next, by subtraction of a hydron. For clarity of names, the ‘added hydrogen’ is cited in names. Preferred IUPAC names are formed by the ‘added indicated hydrogen’ method (see P-58.2).

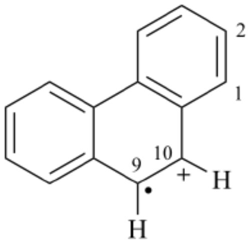
Examples:



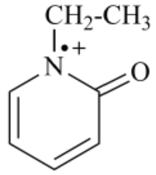
9,10-dihydroanthracen-10-id-9-yl (PIN)



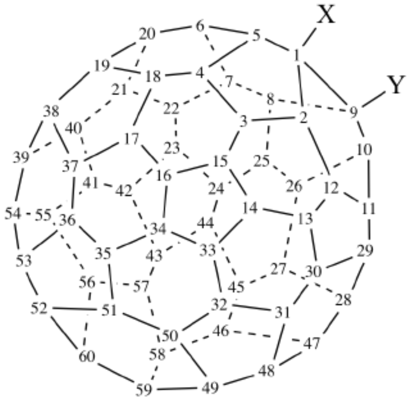
1,4-dihydronaphthalen-4-id-1-yl



9,10-dihydrophenanthren-10-ylium-9-yl (PIN)



1-ethyl-2-oxopyridin-1-ium-1(2*H*)-yl (PIN)
1-ethyl-2-oxo-1,2-dihydropyridin-1-ium-1-yl


X
Y
20
6
5
1
19
18
4
7
8
9
21
22
38
40
3
2
10
17
23
15
25
39
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27
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47
58
60
48
59
49

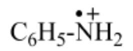
X = • ; Y = +
(C_{60}-*I*$_h$)[5,6]fulleren-9-ylium-1(9*H*)-yl (PIN)
1,9-dihydro(C_{60}-*I*$_h$)[5,6]fulleren-9-ylium-1-yl
X = • ; Y = –
C_{60}-*I*$_h$)[5,6]fulleren-9-id-1(9*H*)-yl (PIN)
1,9-dihydro(C_{60}-*I*$_h$)[5,6]fulleren-9-id-1-yl

P-75.3 RADICAL IONS ON CHARACTERISTIC GROUPS

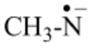
P-75.3.1 Radical ions on ionic suffix groups

When ions may be named by using modified suffixes (see P-73.1.2.1 and P-72.2.2.2.3), the suffixes denoting radical centers are added to the name of the cationic or anionic parent hydride.

Examples:


$C_6H_5\text{-}\overset{\bullet+}{N}H_2$

benzenaminiumyl (PIN)


$CH_3\text{-}\overset{\bullet-}{N}$

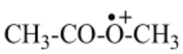
methanaminidyl (PIN)

CH_3-CO-$N^{\bullet+}$
acetamidyliumyl(PIN)

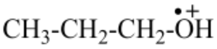
C_6H_5-C≡$N^{\bullet+}$
benzonitriliumyl (PIN)

P-75.3.2 Radical ions other than those named by using ionic suffix groups

Examples:


$CH_3\text{-}CO\text{-}\overset{\bullet+}{O}\text{-}CH_3$

acetyl(methyl)oxidaniumyl (PIN)


$CH_3\text{-}CH_2\text{-}CH_2\text{-}\overset{\bullet+}{O}H$

propyloxidaniumyl (PIN)

$CH_3\text{-}CO\text{-}N^{\bullet -}$
acetylazanidyl (PIN)

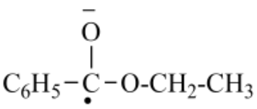
$C_6H_5\text{-}SO_2\text{-}\underset{2}{N}H\text{-}\underset{1}{N}^{\bullet -}$
2-(benzenesulfonyl)hydrazin-1-id-1-yl (PIN)
2-(benzenesulfonyl)diazan-1-id-1-yl

P-75.4 IONIC AND RADICAL CENTERS IN DIFFERENT PARENT STRUCTURES

Radical centers have priority over ionic centers. A radical ion derived formally by the subtraction of one or more hydrogen atom(s) from an ionic or zwitterionic compound in which the ionic and radical centers cannot be included in the same parent structure is named by expressing the ionic center(s), or the part of the structure containing the ionic center(s), by means of substituent prefixes attached to the name of the parent radical.

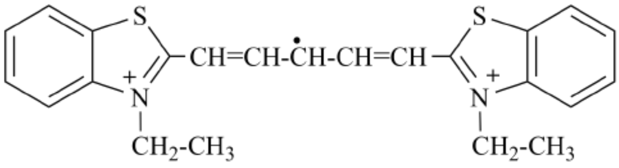
Examples:

$\overset{+}{O}\equiv C\text{-}\overset{\bullet}{C}H_2$
(oxidaniumylidyne)ethyl (PIN)



$C_6H_5-\underset{\bullet}{\overset{\overset{-}{O}}{C}}-O\text{-}CH_2\text{-}CH_3$

ethoxy(oxido)(phenyl)methyl (PIN)
α-ethoxy-α-oxidobenzyl

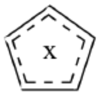


1,5-bis(3-ethyl-1,3-benzothiazol-3-ium-2-yl)penta-1,4-dien-3-yl (PIN)

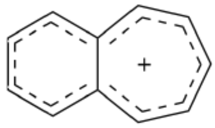
P-76 DELOCALIZED RADICALS AND IONS

Delocalization in names involving one radical or ionic center in an otherwise conjugated double bonds structure is denoted by the appropriate suffix without locants.

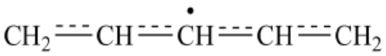
Examples:



x = • : cyclopentadienyl (PIN)
x = + : cyclopentadienylium (PIN)
x = – : cyclopentadienide (PIN)



benzo[7]annulenylium (PIN)



pentadienyl (PIN)

P-77 SALTS

P-77.1 PREFERRED NAMES FOR SALTS OF ORGANIC BASES

P-77.1.1 Preferred IUPAC names for salts of organic bases are binary names formed by citing the name of the cation followed by that of the anion.

Examples:

$C_6H_5\text{-}\overset{+}{N}H_3\ \ Cl^-$
anilinium choride (PIN)
benzenaminium chloride

$$(CH_3\text{-}\overset{+}{N}H_3)_2\quad SO_4^{2-}$$

bis(methanaminium) sulfate (PIN)

$$(CH_3\text{-}CH_2)_3\overset{+}{N}H\quad H^+\quad SO_4^{2-}$$

N,*N*-diethylethanaminium hydrogen sulfate (PIN)

P-77.1.2 Substitutive nomenclature is used to derive preferred IUPAC names for monosalts of di- or polyamines. Adduct names (see P-77.1.3) may be used in general nomenclature.

Example:

$$H_2N\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}H_2\text{-}\overset{+}{N}H_3\quad Cl^-$$

2-aminoethan-1-aminium chloride (PIN)
ethane-1,2-diamine monohydrochloride

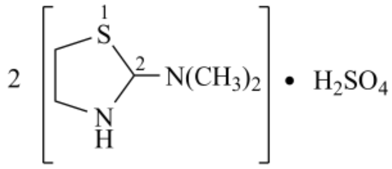
P-77.1.3 When P-77.1.2 cannot be applied, three traditional methods of naming salts of organic bases may be applied as follows:

(1) as adducts. The names of these adducts are preferred IUPAC names only when the acid components of the adducts are organic compounds;

(2) the unaltered name of the base followed by the name of the anion;

(3) for salts of hydrohalogen acids only, the unaltered name of the base is followed by hydrofluoride, hydrobromide, hydrochloride, or hydroiodide, as the case may be.

Example:



(1) *N*,*N*-dimethyl-1,3-thiazolidin-2-amine—sulfuric acid (2/1)
(2) bis(*N*,*N*-dimethyl-1,3-thiazolidin-2-amine) sulfate

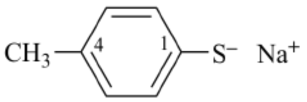
P-77.2 SALTS DERIVED FROM ALCOHOLS (INCLUDING PHENOLS), PEROXOLS, AND THEIR CHALCOGEN ANALOGUES

P-77.2.1 Preferred IUPAC names are binary names formed by citing the name of the cation followed by that of the anion (see P-72.2.2.2.2).

Examples:

$CH_3\text{-}O^-\quad Na^+$

sodium methoxide (PIN)
sodium methanolate



sodium 4-methylbenzene-1-thiolate (PIN)

P-77.2.2 Substitutive nomenclature is used to derive IUPAC preferred names for monosalts of polyhydroxy compounds.

Example:

$HO\text{-}CH_2\text{-}CH_2\text{-}O^-\quad K^+$

potassium 2-hydroxyethan-1-olate (PIN)

P-77.3 SALTS DERIVED FROM ORGANIC ACIDS

P-77.3.1 Preferred IUPAC names are binary names formed by citing the name of the cation followed by that of the anion (see P-72.2.2.2.1).

Example:

$CH_3\text{-}CO\text{-}O^-\quad Na^+$

sodium acetate (PIN)

P-77.3.2 Substitutive nomenclature is used to derive preferred IUPAC names for acid salts of polybasic organic acids (see P-65.6.2.3). In general nomenclature, the hydrogen salt method or a descriptive phrase may be used.

Example:

$$\mathrm{HOOC\text{-}\overset{3}{C}H_2\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}O\text{-}O^- \quad K^+}$$

potassium 3-carboxypropanoate (PIN)
butanedioic acid monopotassium salt

International Union of Pure and Applied Chemistry

Division VIII Chemical Nomenclature and Structure Representation Division

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Chapter P-8 ISOTOPICALLY MODIFIED COMPOUNDS

P-80 Introduction
P-81 Symbols and definitions
P-82 Isotopically substituted compounds
P-83 Isotopically labeled compounds
P-84 Comparative examples of formulas and names of isotopically modified compounds

P-80 INTRODUCTION

This Section describes a general system of nomenclature for organic compounds whose isotopic nuclide composition (refs. 12, 14 and 22) deviates from that occurring in nature (for a discussion of the meaning of 'natural composition' see ref. 29). Examples of isotopic nuclides for hydrogen are given in Table 8.1, below. This Chapter is derived from Section H of the 1979 Recommendations (ref. 1) and Chapter R-8 in the l993 Recommendations (ref. 2). The present Recommendations replace both those of 1979 and 1993. A brief discussion of common biochemical practices can be found in ref. 30.

There is one other system in use for describing isotopically modified compounds. It is based on an extension of the principles proposed by Boughton (see ref. 31) for designating compounds containing hydrogen isotopes and is used mainly in the Chemical Abstracts Service Index Nomenclature system (see ref. 32) for describing isotopic substitution and not isotopic labeling.

The system codified in these recommendations provides for recognition of various types of isotopic modification and thus was chosen in preference to the system based on the Boughton principles which deals only with isotopically substituted compounds.

P-81 SYMBOLS AND DEFINITIONS

P-81.1 NUCLIDE SYMBOLS

The symbol for denoting a nuclide in the formula and name of an isotopically modified compound consists of the atomic symbol for the element and an arabic numeral in the left superscript position indicating the mass number of the nuclide (see IR-3.2, ref.12).

P-81.2 ATOMIC SYMBOLS

The atomic symbols used in the nuclide symbol are those given in IUPAC *Nomenclature of Inorganic Chemistry* (see ref. 12). In the nuclide symbol, the atomic symbol is printed in roman type, italicized atomic symbols being reserved for letter locants, as is customary in the nomenclature of organic compounds and described in P-14.3.

For the hydrogen isotopes protium, deuterium, and tritium, the nuclides symbols ^{1}H, ^{2}H, and ^{3}H, are used. The symbols D and T for ^{2}H and ^{3}H, respectively, are used, but not when other modifying nuclides are present, because this may cause difficulties in alphabetic ordering of the nuclide symbols in the isotopic descriptor.

Although the symbols *d* and *t* have been used and are still used in place of ^{2}H and ^{3}H in names formed according to the Boughton system (see ref 31), in no other cases are only lower-case letters used as atomic symbols. Therefore, the use of *d* and *t* in chemical nomenclature outside of the Boughton system is not recommended.

P-81.3 NAMES FOR HYDROGEN ATOMS AND IONS (see refs. 30, 33)

Table 8.1 Names of the hydrogen atoms and ions

		^1H	**^2H**	**^3H**	**natural composition**
atom	H	protium	deuterium	tritium	hydrogen
anion	H^-	protide	deuteride	tritide	hydride
cation	H^+	proton	deuteron	triton	hydron

P-81.4 ISOTOPICALLY UNMODIFIED COMPOUNDS

An isotopically unmodified compound has a macroscopic composition such that its constituent nuclides are present in the proportions occurring in nature. Its formula and name are written in the customary manner.

Examples:

CH_4
methane

CH_3-CH_2-OH
ethanol

P-81.5 ISOTOPICALLY MODIFIED COMPOUNDS

An isotopically modified compound has a macroscopic composition such that the isotopic ratio of nuclides for at least one element deviates measurably from that occurring in nature. Isotopically modified compounds may be classified as:

(1) isotopically substituted compounds: or

(2) isotopically labeled compounds.

P-82 ISOTOPICALLY SUBSTITUTED COMPOUNDS

P-82.0 Introduction
P-82.1 Structures
P-82.2 Names
P-82.3 Order of nuclide symbols
P-82.4 Stereoisomeric isotopically substituted compounds
P-82.5 Numbering
P-82.6 Locants

P-82.0 INTRODUCTION

An isotopically substituted compound has a composition such that essentially all the molecules of the compound have only the indicated nuclide at each designated position. For all other positions, the absence of nuclide indication means that the nuclide composition is the natural one.

P-82.1 STRUCTURES

The structure of an isotopically substituted compound is written in the usual way except that appropriate nuclides symbols are used. When different isotopes of the same element are present in the same position, their symbols are written in order of increasing mass number.

Examples:

$^{14}CH_4$

$^{12}CHCl_3$

CH_3-CH^2H-OH
(not CH_3-C^2HH-OH)

P-82.2 NAMES

P-82.2.1 The name of an isotopically substituted compound is formed by adding or inserting the nuclide symbol(s) enclosed in parentheses, preceded by any necessary locant(s), letters, and/or numerals, before the part of the compound that is isotopically substituted. Immediately after the parentheses there is neither space nor hyphen, except that when the name, or a part of a name, includes a preceding locant, a hyphen is inserted. When two or more nuclide symbols appear at the same place in the name they are cited first in alphabetical order and then by their mass number, if necessary (see P-82.3)

When polysubstitution at a single position is possible, the number of atoms substituted is always specified as a right subscript to the atomic symbol(s), even in case of monosubstitution. For polysubstitution with isotopically modified and unmodified atoms or groups, see P-82.2.2. For compounds modified by hydro prefixes, see P-82.2.3.

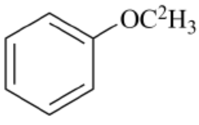
Examples:

$^{14}CH_4$
(^{14}C)methane (PIN)

$^{12}CHCl_3$
trichloro(^{12}C)methane (PIN)
(^{12}C)chloroform

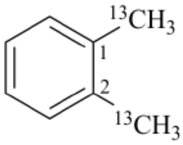
$CH_3{}^2H$
$(^2H_1)$methane (PIN)

$C^2H_2Cl_2$
dichloro$(^2H_2)$methane (PIN)

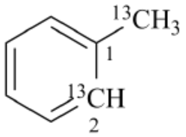


$(^2H_3)$methoxybenzene (PIN)
$(\alpha,\alpha,\alpha\text{-}^2H_3)$anisole

$C_6H_5\text{-}^{13}CO\text{-}^{13}CH_3$
1-phenyl$(1,2\text{-}^{13}C_2)$ethan-1-one (PIN)
$(1,2\text{-}^{13}C_2)$acetophenone



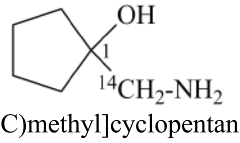
1,2-di[(^{13}C)methyl]benzene (PIN)
$(\alpha,\alpha'\text{-}^{13}C_2)$-1,2-xylene
$(\alpha,\alpha'\text{-}^{13}C_2)$-*o*-xylene



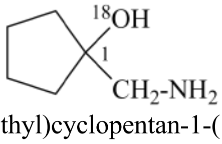
1-(^{13}C)methyl$(2\text{-}^{13}C)$benzene (PIN)
$(\alpha,2\text{-}^{13}C_2)$-toluene

$CH_2{}^2H\text{-}CH_2\text{-}OH$
(2-^2H_1)ethan-1-ol (PIN)

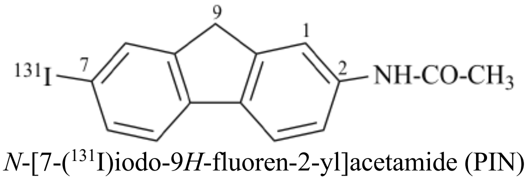
$^{13}CH_3\text{-}CH_2\text{-}OH$
$(2\text{-}^{13}C)$ethan-1-ol (PIN)



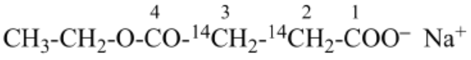
1-[amino(^{14}C)methyl]cyclopentan-1-ol (PIN)



1-(aminomethyl)cyclopentan-1-(^{18}O)ol (PIN)

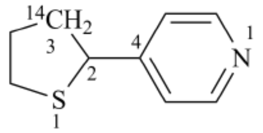


N-[7-(^{131}I)iodo-9*H*-fluoren-2-yl]acetamide (PIN)

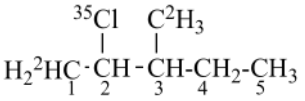


$\overset{4}{\mathrm{CH_3\text{-}CH_2\text{-}O\text{-}CO}}\text{-}\overset{3}{\mathrm{^{14}CH_2}}\text{-}\overset{2}{\mathrm{^{14}CH_2}}\text{-}\overset{1}{\mathrm{COO^-}}\ \mathrm{Na^+}$

sodium 4-ethoxy-4-oxo(2,3-$^{14}C_2$)butanoate (PIN)
sodium ethyl (2,3-$^{14}C_2$)butanedioate
sodium ethyl (2,3-$^{14}C_2$)succinate



4-[(3-^{14}C)thiolan-2-yl]pyridine (PIN)
4-[tetrahydro(3-^{14}C)thiophen-2-yl]pyridine



$\mathrm{H_2{}^2HC\text{-}CH(^{35}Cl)\text{-}CH(C^2H_3)\text{-}CH_2\text{-}CH_3}$

2-(^{35}Cl)chloro-3-($^2H_3$)methyl(1-$^2H_1$)pentane (PIN)

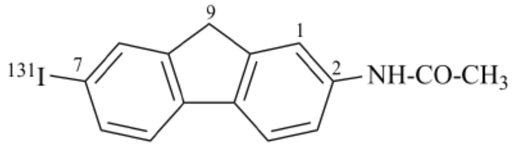
P-82.2.2 The name of an isotopically modified compound may differ from the name of the unmodified analogue when its structure contains identical units that are not identically modified in equivalent positions. Such different groups are expressed separately.

> Isotopically modified atoms or groups that are not identically modified in equivalent positions are expressed separately, which is a change from Section H of the 1979 Recommendations (ref. 1) and Chapter R-8 of the l993 Recommendations (ref. 2).

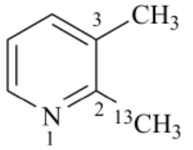
P-82.2.2.1 Different isotopic modifications on otherwise identical substituents

When two substituent groups are isotopically modified in different ways so that they cannot be combined together using multiplicative terns such as 'di-', 'bis-', etc., they are cited separately. The isotopically modified substituent is preferred alphabetically to the unmodified substituent.

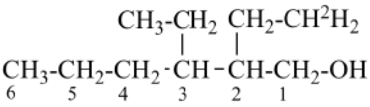
Examples:



N-[7-(^{131}I)iodo-6-iodo-9*H*-fluoren-2-yl]acetamide (PIN)
{not *N*-[6,7-(7-^{131}I)diiodo-9*H*-fluoren-2-yl]acetamide}



2-(^{13}C)methyl-3-methylpyridine (PIN)
[not 2,3-(2-^{13}C)dimethylpyridine]

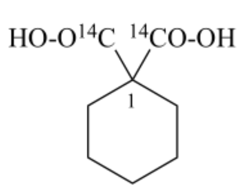


$\mathrm{CH_3\text{-}CH_2\text{-}CH_2\text{-}CH(CH_2\text{-}CH_3)\text{-}CH(CH_2\text{-}CH^2H_2)\text{-}CH_2\text{-}OH}$

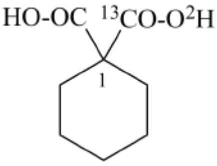
2-(2,2-$^2H_2$)ethyl-3-ethylhexan-1-ol (PIN)

P-82.2.2.2 When two characteristic groups are isotopically modified in different ways so that they cannot be combined using multiplicative terms such as 'di-', 'bis-', etc., the isotopically modified characteristic group with the greater number of modifications is chosen as the principal characteristic group to be cited as a suffix; the other characteristic is then cited as a prefix. If a further choice is needed, the suffix with the nuclide of higher atomic number, then the nuclide of higher mass number, is chosen as the principal characteristic group to be cited as a suffix.

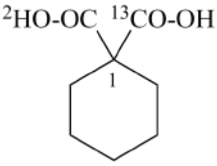
Examples:



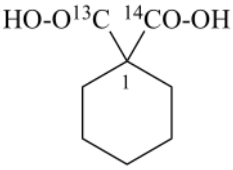
cyclohexane-1,1-di[(^{14}C)carboxylic acid] (PIN)



1-carboxycyclohexane-1-(^{13}C,^{2}H)carboxylic acid (PIN)



1-(^{2}H)carboxycyclohexane-1-(^{13}C)carboxylic acid (PIN)



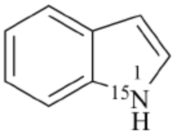
1-(^{13}C)carboxycyclohexane-1-(^{14}C)carboxylic acid (PIN)

P-82.2.3 Addition of hydro prefixes

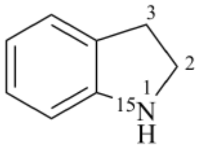
Isotopically modified hydrogen atoms, when present, are always attached to the skeleton of the isotopically modified compound. According to P-82.2.2, the hydro prefixes must be identical, whether unmodified or isotopically modified, and added in pairs. Isotopically modified or unmodified hydro prefixes are added as detachable substituent prefixes placed at the front of the parent hydride.

In these recommendations hydrogenated mancude ring systems are treated as described in P-82.2.2 which is a change from previous recommendations.

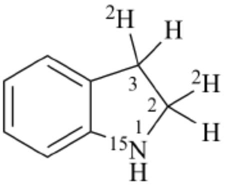
Examples:



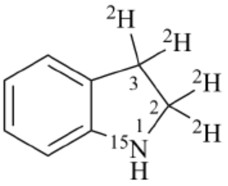
(^{15}N)-1*H*-indole (PIN)



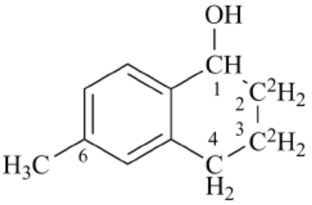
2,3-dihydro(^{15}N)-1*H*-indole (PIN)



2,3-dihydro(2,3-^{2}H$_{2}$,^{15}N)-1*H*-indole (PIN)



2,3-di[(^{2}H)hydro](2,3-^{2}H$_{2}$,^{15}N)-1*H*-indole (PIN)
[not (2,3-^{2}H$_{2}$)dihydro(2,3-^{2}H$_{2}$,1-^{15}N)-1*H*-indole]



6-methyl-2,3-di[(^{2}H)hydro]-1,4-dihydro(2,3-$^{2}H_2$)naphthalen-1-ol (PIN)
{not 6-methyl-1,4-dihydro-2,3-di[(^{2}H)hydro](2,3-$^{2}H_2$)naphthalen-1-ol;
not 6-methyl[(2,3-$^{2}H_2$)-1,2,3,4-tetrahydro](2,3-$^{2}H_2$)naphthalen-1-ol;
these names do not conform to P-82.2.2}

P-82.2.4 In a name consisting of two or more words, the isotopic descriptor is placed before the appropriate word or part of the word that includes the nuclide(s), unless unambiguous locants are available or are unnecessary.

Examples:

$\overset{2}{C}H_2{}^2H\text{-}\overset{1}{C}OOH$
(2-$^{2}H_1$)acetic acid (PIN)

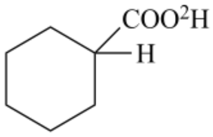
$CH_3\text{-}COO{}^2H$
(O-^{2}H)acetic acid (PIN)
acetic (^{2}H)acid

$CH_3\text{-}C{}^{18}O\text{-}O{}^2H$
(O-^{2}H,^{18}O)acetic acid (PIN)

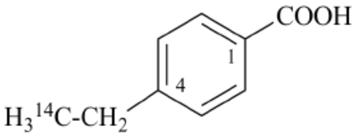
$CH_3\text{-}CO\text{-}{}^{18}O{}^2H$
(^{18}O-^{2}H,^{18}O)acetic acid (PIN)

$\overset{5}{C}H_3\text{-}\overset{4}{C}H_2\text{-}\overset{3}{C}H_2\text{-}\overset{2}{C}H_2\text{-}{}^{14}\overset{1}{C}OO{}^3H$
(1-^{14}C)pentan(^{3}H)oic acid (PIN)

$H{}^{14}COO^- \ Na^+$
sodium (^{14}C)formate (PIN)



cyclohexane(^{2}H)carboxylic acid (PIN)



4-(2-^{14}C)ethylbenzoic acid (PIN)

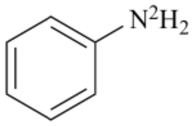
$CH_3\text{-}CH_2\text{-}COO\text{-}{}^{14}\overset{1}{C}H_2\text{-}\overset{2}{C}H_3$
(1-^{14}C)ethyl propanoate (PIN)

$\overset{3}{C}H_3\text{-}{}^{14}\overset{2}{C}H_2\text{-}\overset{1}{C}OO\text{-}CH_2\text{-}CH_3$
ethyl (2-^{14}C)propanoate (PIN)

P-82.2.5 In a name consisting of one word, the isotopic descriptor is placed before the name, with an appropriate locant. This method is preferred to that of placing the descriptor before the implied name of the characteristic group.

Examples:

$CH_3\text{-}CO\text{-}\overset{N}{N}H{}^2H$
(N-$^{2}H_1$)acetamide (PIN)



(N-$^2H_2$)aniline (PIN)
(N-$^2H_2$)benzenamine

P-82.3 ORDER OF NUCLIDE SYMBOLS

P-82.3.1 When isotopes of different elements are present as nuclides in an isotopically substituted compound, their symbols are arranged in alphabetical order if they are at the same place in the name.

Example:

$CH_3{}^{18}O^2H$
methan(^2H,^{18}O)ol (PIN)

P-82.3.2 When several isotopes of the same element are present as nuclides in an isotopically substituted compound, their symbols are arranged in the order of increasing mass number if they are inserted at the same place in the name.

Example:

$\overset{2}{C}H_2{}^2H\text{-}\overset{1}{C}H^3H\text{-}OH$
(2-$^2H_1$,1-$^3H_1$)ethan-1-ol (PIN)

P-82.4 STEREOISOMERIC ISOTOPICALLY SUBSTITUTED COMPOUNDS

Two types of stereoisomeric isotopically substituted compounds are possible:

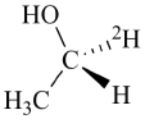
(1) those in which the stereoisomerism results from isotopic modification;

(2) those whose analogous unmodified compounds are themselves stereoisomers.

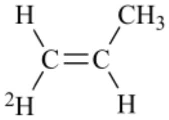
The nomenclature for stereoisomers of isotopically substituted compounds follows the general methods described in Chapter P-9.

Stereodescriptors are cited at the specified place in the name according to the stereochemical rules. When they must be inserted into the name at the same place as isotopic descriptors, the stereodescriptors are cited first.

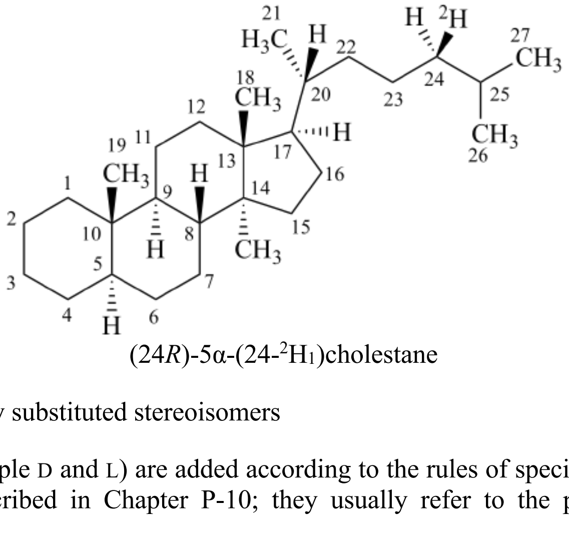
P-82.4.1 Examples in which stereoisomerism results from isotopic substitution



(1*R*)-(1-$^2H_1$)ethan-1-ol (PIN)



(1*E*)-(1-$^2H_1$)prop-1-ene (PIN)

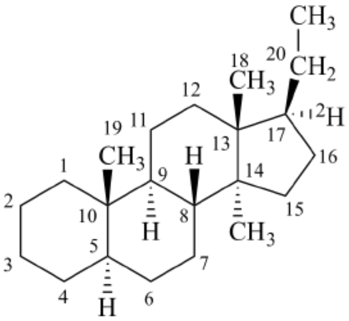


(24*R*)-5α-(24-$^2H_1$)cholestane

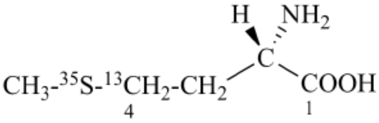
P-82.4.2 Examples of isotopically substituted stereoisomers

Stereochemical affixes (for example D and L) are added according to the rules of special classes, such as carbohydrates, amino acids, steroids, etc., described in Chapter P-10; they usually refer to the parent substance (or unmodified compound) according to the particular class of compounds. In these classes isotopic descriptors may follow the stereochemical descriptors according to biochemical usage (ref. 30).

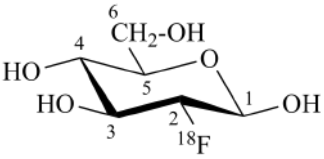
Examples:



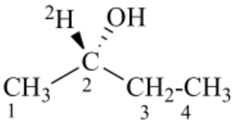
5α-(17-^{2}H)pregnane



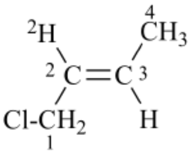
L-(4-^{13}C,^{35}S)methionine



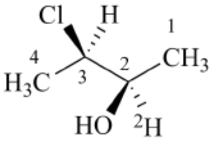
2-deoxy-2-(^{18}F)fluoro-β-D-glucopyranose



(2*S*)-(2-^{2}H)butan-2-ol (PIN)



(2*E*)-1-chloro(2-^{2}H)but-2-ene (PIN)



(2*R*,3*R*)-3-chloro(2-^{2}H)butan-2-ol (PIN)

P-82.5 NUMBERING

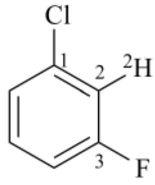
P-82.5.1 Numbering in relation to the unmodified compound

Numbering of an isotopically substituted compound is not changed from that of an isotopically unmodified compound. Among the structural features of a compound to be considered successively for numbering as given by P-14.4, the presence of nuclides is considered last with the exception of chirality arising from isotopic modification.

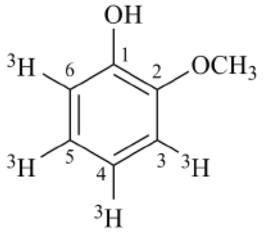
Examples:

$$\overset{1}{C}F_3\text{-}\overset{2}{C}H_2{}^2H$$

1,1,1-trifluoro(2-^{2}H$_1$)ethane (PIN)



1-chloro-3-fluoro(2-^{2}H)benzene (PIN)

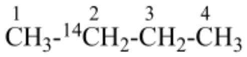


2-methoxy(3,4,5,6-$^{3}H_4$)phenol (PIN)

P-82.5.2 Priority between isotopically substituted and unmodified atoms or groups

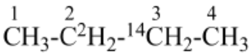
When there is a choice between equivalent numberings in an isotopically unmodified compound, the starting point and the direction of numbering of the analogous isotopically substituted compound are chosen so as to give lowest locants to the modified atoms or groups considered together in one series in increasing numerical order. If a choice still remains, precedence for the lowest locants is given to the nuclide of higher atomic number. In the case of different nuclides of the same element, precedence is given to the nuclide of higher mass number.

Examples:



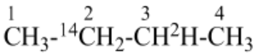
$\overset{1}{C}H_3\text{-}{}^{14}\overset{2}{C}H_2\text{-}\overset{3}{C}H_2\text{-}\overset{4}{C}H_3$

(2-^{14}C)butane (PIN)
[not (3-^{14}C)butane]



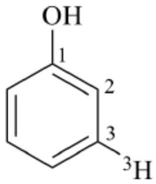
$\overset{1}{C}H_3\text{-}\overset{2}{C}{}^{2}H_2\text{-}{}^{14}\overset{3}{C}H_2\text{-}\overset{4}{C}H_3$

(3-^{14}C,2,2-$^{2}H_2$)butane (PIN)
[not (2-^{14}C,3,3-$^{2}H_2$)butane]

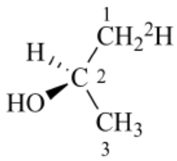


$\overset{1}{C}H_3\text{-}{}^{14}\overset{2}{C}H_2\text{-}\overset{3}{C}H{}^{2}H\text{-}\overset{4}{C}H_3$

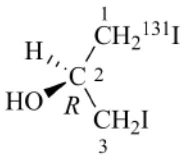
(2-^{14}C,3-$^{2}H_1$)butane (PIN)
[not (3-^{14}C,2-$^{2}H_1$)butane]



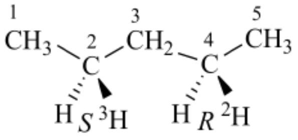
(3-^{3}H)phenol (PIN)



(2*R*)-(1-$^{2}H_1$)propan-2-ol (PIN)



(2*R*)-(1-^{131}I)iodo-3-iodopropan-2-ol (PIN)



(2*S*,4*R*)-(4-$^{2}H_1$,2-$^{3}H_1$)pentane (PIN)

P-82.6 LOCANTS

P-82.6.1 Omission of locants (see also P-14.3.4)

P-82.6.1.1 In preferred IUPAC names, locants are omitted if no locants are necessary in unmodified names. However, if isotopic modification requires a locant to specify its position, then all locants must be specified and none are omitted.

Examples:

$C^{2}H_{3}\text{-}CN$
(^{2}H$_{3}$)acetonitrile (PIN)
(as in trichloroacetonitrile)

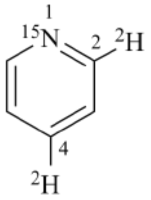
$CH_{3}\text{-}CH_{2}\text{-}O^{2}H$
ethan(^{2}H)ol (PIN)
(as in ethanol)

$^{13}CH_{3}\text{-}CH_{2}\text{-}OH$
(2-^{13}C)ethan-1-ol
[not (2-^{13}C)ethanol]

$CH_{2}{}^{2}H\text{-}O\text{-}C^{2}H_{2}\text{-}S\text{-}CH_{2}\text{-}OOH$
{[(^{2}H$_{1}$)methoxy(^{2}H$_{2}$)methyl]sulfanyl}methaneperoxol (PIN)

P-82.6.1.2 Locants are omitted when there is only one atom of a given element.

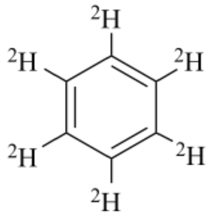
Example:



(2,4-^{2}H$_{2}$,^{15}N)pyridine (PIN)

P-82.6.1.3 Locants are omitted in compounds or substituent groups in which all positions are completely isotopically substituted or modified in the same way.

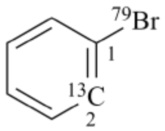
Example:



(^{2}H$_{6}$)benzene (PIN)

P-82.6.1.4 Locants are not omitted when there is a possibility of isomers

Example:



1-(^{79}Br)bromo(2-^{13}C)benzene (PIN)

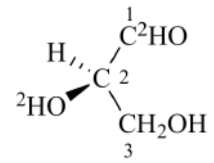
P-82.6.2 Letter and/or numeral locants

When locants are needed for defining the structure of the parent structure or of a unit of structure as defined by its appropriate enclosing marks, then all locants must be cited for the parent structure or that structural unit. Specific positions of nuclides must be indicated in the isotopic descriptor by appropriate locants, letters, and/or numerals, preceding the nuclide symbol(s). In preferred names, all locants are placed before the nuclide that is multiplied.

Examples:

$CH_{3}\text{-}CH^{2}H\text{-}O^{2}H$
(1-^{2}H$_{1}$)ethan-1-(^{2}H)ol (PIN)

$\overset{1}{C^{2}H_{3}}\text{-}\overset{2}{CO}\text{-}\overset{3}{C^{2}H_{2}}\text{-}\overset{4}{CH_{2}}\text{-}\overset{5}{CH_{3}}$
(1,1,1,3,3-^{2}H$_{5}$)pentan-2-one (PIN)

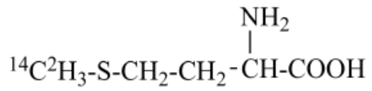


(2*R*)-2-(^{2}H)hydroxy-3-hydroxy(1-^{2}H)propanal (PIN)
D-(2-*O*,1-$^{2}H_2$)glyceraldehyde

P-82.6.3 Location of nuclides on positions not normally denoted by locants

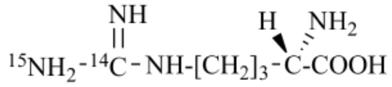
P-82.6.3.1 When a nuclide occupies a position that is not numbered, an italicized prefix or Greek letter may be used to denote its position.

Examples:



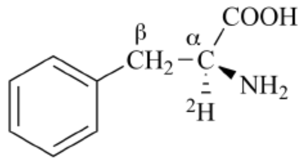
$^{14}C^{2}H_3\text{-S-}CH_2\text{-}CH_2\text{-}\overset{NH_2}{\overset{|}{C}}H\text{-COOH}$

DL-[*methyl*-(^{14}C,$^{2}H_3$)]methionine



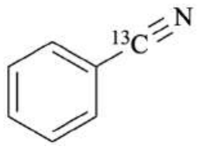
$^{15}NH_2\text{-}^{14}\overset{NH}{\overset{||}{C}}\text{-NH-}[CH_2]_3\text{-}\overset{H\ \ NH_2}{C}\text{-COOH}$

L-(*carbamimidoyl*-^{14}C,*N*′-^{15}N)arginine
L-(*guanidino*-^{14}C,*N*′-^{15}N)arginine (see Rule H-4.21, ref. 1)
(not L-(*amidino*-^{14}C,*N*′-^{15}N)arginine)

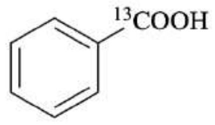


L-(α-^{2}H)phenylalanine

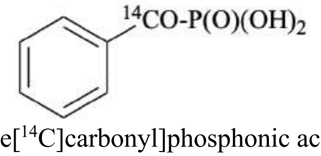
P-82.6.3.2 When the nuclide is located at a position in a retained name that is not numbered a systematic name that identifies separately the relevant atom is used for the IUPAC preferred name. For general nomenclature an italicized prefixes or Greek letters may be used to denote its position.



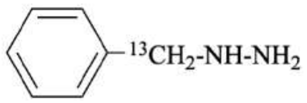
benzene(^{13}C)carbonitrile (PIN)
(*cyano*-^{13}C)benzonitrile



benzene(^{13}C)carboxylic acid (PIN)
(*carboxyl*-^{13}C)benzoic acid



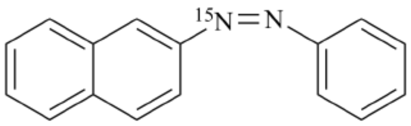
[benzene[^{14}C]carbonyl]phosphonic acid (PIN)
[phenyl[^{14}C]carbonyl]phosphonic acid
[*carbonyl*-^{14}C]benzoylphosphonic acid



[phenyl(^{13}C)methyl]hydrazine (PIN)
[(α-^{13}C)benzyl]hydrazine

P-82.6.3.3 When a nuclide occupies a position that is not numbered or when its position cannot be easily defined according to rule P-82.6.3.1, the nuclide symbol is included in the entire symbol of the group through which it is linked to the main part of the structure. This rule is useful in general nomenclature in which many names are constructed without locants.

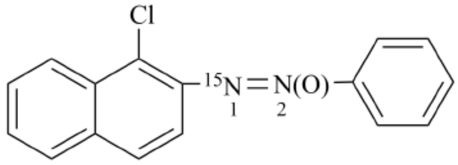
Examples:



1-(naphthalen-2-yl)-2-phenyl(1-^{15}N)diazene (PIN)
naphthalene-2-(^{15}N=N)azobenzene

CH_3-CH_2-CH=^{15}N-NH_2
1-propylidene(1-^{15}N)hydrazine (PIN)
propanal (^{15}N-NH_2)hydrazone

$CH_3\text{-}CH_2\text{-}S\text{-}{}^{34}S\text{-}S\text{-}\overset{3}{C}H_2\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}OOH$
3-[ethyl(2-^{34}S)trisulfanyl]propanoic acid (PIN)
3-[ethyl(S-^{34}S-S)trithio]propionic acid (see Rule H-4.22. ref. 1)



1-(1-chloronaphthalen-2-yl)-2-phenyl(1-^{15}N)diazene 2-oxide (PIN)
1-chloro-2-(phenyl-*ON*^{15}*N*-azoxy)naphthalene

P-82.6.4 Italicized nuclide symbols and/or italic capital letters are used to distinguish between different nuclides of the same element.

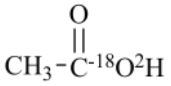
Examples:

CH_3-CH_2-CO-^{18}O-CH_2-CH_3
^{18}*O*-ethyl propan($^{18}O_1$)oate (PIN)

CH_3-CH_2-C^{18}O-O-CH_2-CH_3
O-ethyl propan($^{18}O_1$)oate (PIN)

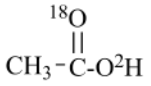
CH_3-O-CO-^{18}O-CH_2-CH_3
^{18}*O*-ethyl *O*-methyl ($^{18}O_1$)carbonate (PIN)

CH_3-CH_2-O-C^{18}O-^{18}O-CH_3
O-ethyl ^{18}*O*-methyl ($^{18}O_2$)carbonate (PIN)



$CH_3\text{-}\overset{\overset{\displaystyle O}{||}}{C}\text{-}{}^{18}O^2H$

(^{18}*O*-^{2}H,^{18}O)acetic acid (PIN)



$CH_3\text{-}\overset{\overset{\displaystyle {}^{18}O}{||}}{C}\text{-}O^2H$

(*O*-^{2}H,^{18}O)acetic acid (PIN)
(the '^{18}O' is an isotopic descriptor and the '*O*' is a locant)

P-83 ISOTOPICALLY LABELED COMPOUNDS

An isotopically labeled compound is a mixture of isotopically unmodified compound with one or more analogous isotopically substituted compound(s).

Although an isotopically labeled compound is really a mixture as far as chemical identity is concerned (in the same way as is an unmodified compound), for nomenclature purposes, such mixtures are called 'isotopically labeled' compounds.

P-83.1 Specifically labeled compounds
P-83.2 Selectively labeled compounds
P-83.3 Nonselectively labeled compounds
P-83.4 Isotopically deficient compounds
P-83.5 General and uniform labeling

P-83.1 SPECIFICALLY LABELED COMPOUNDS

An isotopically labeled compound is designated as ‘specifically labeled’ when a unique isotopically substituted compound is formally added to the analogous isotopically unmodified compound. In such a case, both position(s) and number of nuclides are defined.

Structures (see P-83.1.1) are identical to those given in Section P-82 for isotopically substituted compounds, except that brackets enclose the nuclide symbol.

Examples:

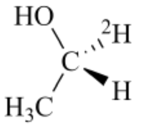
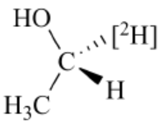
Isotopically substituted compound	**when added to**	**Isotopically unmodified compound**	**gives rise to**	**Specifically labeled compound**
$^{13}CH_4$		CH_4		$[^{13}C]H_4$
$CH_2{}^2H_2$		CH_4		$CH_2[^2H_2]$

P-83.1.1 Structures of specifically labeled compounds

The structural formula of a specifically labeled compound is written in the usual way, but with the appropriate nuclide symbol(s) and multiplying subscript enclosed in square brackets, [ ]. The structural formula is written in the same way as that of an isotopically substituted compound.

Although the formula for a specifically labeled compound does not represent the composition of the bulk material, which usually consists overwhelmingly of the isotopically unmodified compound, it does indicate the presence of the compound of chief interest, the isotopically substituted compound.

Examples:

Formulas of isotopically substituted compounds	**Formulas of specifically labeled compounds**
$CH_3\text{-}CO\text{-}NH^2H$	$CH_3\text{-}CO\text{-}NH[^2H]$
	
$C^2H_3\text{-}CO\text{-}C^2H_2\text{-}CH_2\text{-}CH_3$	$C[^2H_3]\text{-}CO\text{-}C[^2H_2]\text{-}CH_2\text{-}CH_3$

A specifically labeled compound is:

(a) singly labeled when the isotopically substituted compound has only one isotopically modified atom;

Example:

$CH_3\text{-}CH[^2H]\text{-}OH$

(b) multiply labeled when the isotopically substituted compound has more than one modified atom of the same element at the same position or at different positions;

Examples:

$CH_3\text{-}C[^2H_2]\text{-}OH$

$CH_2[^2H]\text{-}CH[^2H]\text{-}OH$

(c) mixed labeled when the isotopically substituted compound has more than one kind of modified atom.

Example:

$CH_3\text{-}CH_2\text{-}[^{18}O][^2H]$

P-83.1.2 Names of specifically labeled compounds

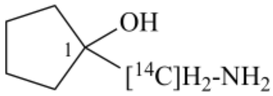
P-83.1.2.1 The name of a specifically labeled compound is formed by adding or inserting in brackets, [ ], the nuclide symbol(s) preceded by any necessary locants before the denomination of that part of the compound that is isotopically modified. When polylabeling is possible, the number of atoms that have been labeled is always specified as a subscript to the atomic symbol(s) even in the case of monolabeling. This is necessary in order to distinguish between a specifically and a selectively or nonselectively labeled compound.

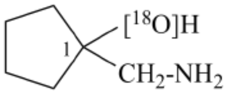
Examples:

$[^{13}C]H_4$
[^{13}C]methane (PIN)

$CH_3[^{2}H]$
[$^{2}H_1$]methane (PIN)

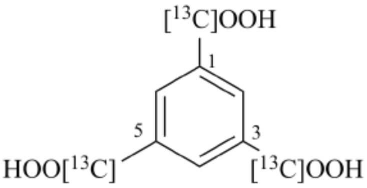
$C[^{2}H_2]Cl_2$
dichloro[$^{2}H_2$]methane (PIN)

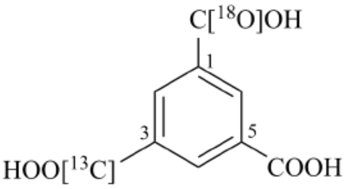

OH
1
[14C]H2-NH2
1-(amino[^{14}C]methyl)cyclopentan-1-ol (PIN)

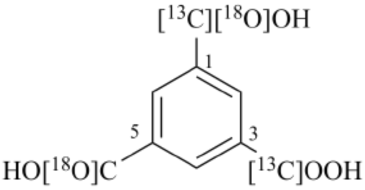

[18O]H
1
CH2-NH2
1-(aminomethyl)cyclopentan-1-[^{18}O]ol (PIN)

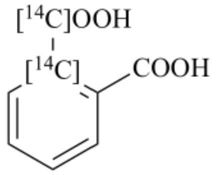
P-83.1.2.2 All rules given in P-82 to construct names of isotopically substituted compounds are applicable to construct names of specifically labeled compounds, with the exception that the isotopic descriptor is placed in brackets and parentheses are used around complex prefixes. For examples of geminal dicarboxylic acids, see P-82.2.2.2.

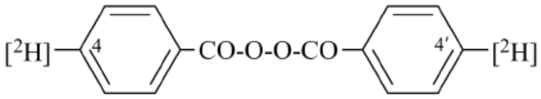
Examples:


[13C]OOH
1
5
3
HOO[13C]
[13C]OOH
benzene-1,3,5-tri([^{13}C]carboxylic acid) (PIN)
(not benzene-1,3,5-[1,3,5-$^{13}C_3$]tricarboxylic acid)

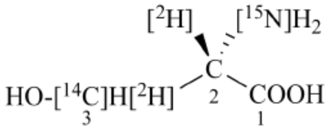

C[18O]OH
1
3
5
HOO[13C]
COOH
3-[^{13}C]carboxy-5-carboxybenzene-1-[^{18}O]carboxylic acid (PIN)
(not benzene-1,3,5-[3-^{13}C,1-^{18}O]tricarboxylic acid)


[13C][18O]OH
1
5
3
HO[18O]C
[13C]OOH
3-[^{13}C]carboxy-5-[^{18}O]carboxybenzene-1-[^{13}C,^{18}O]carboxylic acid (PIN)
(not benzene-1,3,5-[1,3-$^{13}C_2$,1,5-$^{18}O_2$]tricarboxylic acid)

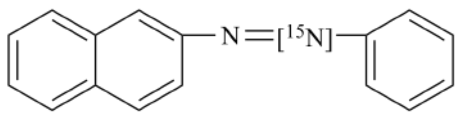

[14C]OOH
[14C]
COOH
2-carboxy[1-^{14}C]benzene-1-[^{14}C]carboxylic acid (PIN)
(not [1-^{14}C]benzene-1,2-[1-^{14}C]dicarboxylic acid)
[1-^{14}C]phthalic [1-^{14}C]acid


[2H]
4
CO-O-O-CO
4′
[2H]
di([4-^{2}H]benzoyl) peroxide
[4-^{2}H]benzoic peroxyanhydride (PIN)

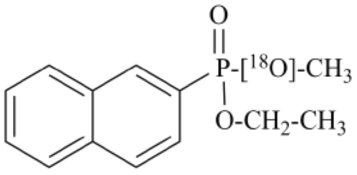
$CH_3\text{-}[^{14}C]OOH$
[1-^{14}C]acetic acid (PIN; see P-82.2.4)



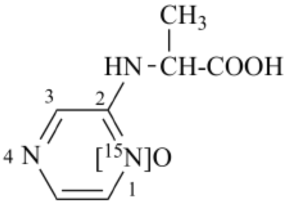
L-[3-^{14}C,2,3-$^{2}H_2$,^{15}N]serine (see P-82.4.2)
(2*S*)-2-[^{15}N]amino-3-hydroxy[2,3-$^{2}H_2$,3-^{14}C]propanoic acid



1-(naphthalen-2-yl)-2-phenyl[2-^{15}N]diazene (PIN)
naphthalene-2-[N=^{15}N]azobenzene (see P-82.6.3.3)



O-ethyl ^{18}*O*-methyl (naphthalen-2-yl)[^{18}O]phosphonate (PIN) (see P-82.6.4)



2-[(1-carboxyethyl)amino][1-^{15}N]pyrazine 1-oxide
N-([1-^{15}N]pyrazin-2-yl)alanine ^{15}*N*-oxide (see P-82.6.4)

P-83.2 SELECTIVELY LABELED COMPOUNDS

An isotopically labeled compound is designated as selectively labeled when a mixture of isotopically substituted compounds is formally added to the analogous isotopically unmodified compound in such a way that the position(s) but not necessarily the number of each labeling nuclide is defined. A selectively labeled compound may be considered as a mixture of specifically labeled compounds. A selectively labeled compound may be:

(a) multiply labeled when in the unmodified compound there is more than one atom of the same element at the position where the isotopic modification occurs, for example H, in CH_4; or there are several atoms of the same element at different positions where the isotopic modification occurs, for example C, in C_4H_8O;

(b) mixed labeled when there is more than one labeling nuclide in the compound, for example, C and O in CH_3-CH_2-OH.

When there is only one atom of an element that can be modified in a compound, only specific labeling can result.

P-83.2.1 Structures of selectively labeled compounds

P-83.2.1.1 A selectively labeled compound cannot be described by a unique structural formula; therefore it is represented by inserting the nuclide symbol(s) preceded by any necessary locant(s) (letters and/or numbers) but without multiplying subscripts, enclosed in square brackets, [ ], directly before the usual formula or, if necessary, before parts of the formula that have an independent numbering. Identical locants are not repeated. When different nuclides are present, the nuclide symbols are written in alphabetical order according to their symbols, or when the atomic symbols are identical, in order of increasing mass number.

Examples:

Mixture of	**when**	**Isotopically**	**gives**	**Selectively**

isotopically substituted compounds	added to	unmodified compound	rise to	labeled compound
$CH_3{}^2H$, $CH_2{}^2H_2$ CH^2H_3, C^2H_4 or any two or more of the above		CH_4		$[^2H]CH_4$
$\overset{4}{C}H_3-\overset{3}{C}H_2-\overset{2}{C}H^2H-\overset{1}{C}OOH$ $\overset{4}{C}H_3-\overset{3}{C}H_2-\overset{2}{C}{}^2H_2-\overset{1}{C}OOH$		$CH_3-CH_2-CH_2-COOH$		$[2-^2H]\overset{4}{C}H_3-\overset{3}{C}H_2-\overset{2}{C}H_2-\overset{1}{C}OOH$
$\overset{4}{C}H_3-{}^{14}\overset{3}{C}H_2-{}^{14}\overset{2}{C}H_2-\overset{1}{C}OOH$ $\overset{4}{C}H_3-{}^{14}\overset{3}{C}H_2-\overset{2}{C}H_2-\overset{1}{C}OOH$ $\overset{4}{C}H_3-\overset{3}{C}H_2-{}^{14}\overset{2}{C}H_2-\overset{1}{C}OOH$ or any two of the above		$CH_3-CH_2-CH_2-COOH$		$[2,3-^{14}C]\overset{4}{C}H_3-\overset{3}{C}H_2-\overset{2}{C}H_2-\overset{1}{C}OOH$
$\overset{2}{C}H_3-{}^{14}\overset{1}{C}H_2-OH$ $\overset{2}{C}H_3-\overset{1}{C}H_2-{}^{18}OH$ $\overset{2}{C}H_3-{}^{14}\overset{1}{C}H_2-{}^{18}OH$ or any two of the above		CH_3-CH_2-OH		$[2,3-^{14}C]\overset{4}{C}H_3-\overset{3}{C}H_2-\overset{2}{C}H_2-\overset{1}{C}OOH$
${}^{14}\overset{3}{C}H_3-\overset{2}{C}H_2-\overset{1}{C}OO-CH_3$ ${}^{14}\overset{3}{C}H_3-\overset{2}{C}H_2-\overset{1}{C}OO-{}^{14}CH_3$ $\overset{3}{C}H_3-\overset{2}{C}H_2-\overset{1}{C}OO-{}^{14}CH_3$ or any two of the above		$CH_3-CH_2-COO-CH_3$		$[3-^{14}C]\overset{3}{C}H_3-\overset{2}{C}H_2-\overset{1}{C}OO-[^{14}C]CH_3$

P-83.2.1.2 In a selectively labeled compound formally arising from mixing several known isotopically substituted compounds with the analogous isotopically unmodified compound, the number or the possible number of labeling nuclide(s) for each position may be indicated by subscripts to the atomic symbol(s). Two or more subscripts referring to the same nuclide symbol are separated by a semicolon. For a multiply labeled or mixed labeled compound, the subscripts are written successively in the same order as the various isotopically substituted compounds are considered. The subscript zero is used to indicate that one of the isotopically substituted compounds is not modified at the indicated position.

Examples:

Mixture of isotopically substituted compound	when added to	Isotopically unmodified compound	gives rise to	Selectively labeled compound
$\overset{2}{C}H_2{}^2H-\overset{1}{C}H_2-OH$ $\overset{2}{C}H^2H_2-\overset{1}{C}H_2-OH$		CH_3-CH_2-OH		$[2-^2H_{1;2}]\overset{2}{C}H_3-\overset{1}{C}H_2-OH$
$\overset{2}{C}H^2H_2-\overset{1}{C}H_2-OH$ $\overset{2}{C}H^2H_2-\overset{1}{C}H_2-{}^{18}OH$		CH_3-CH_2-OH		$[2-^2H_{2;2},^{18}O_{0;1}]\overset{2}{C}H_3-\overset{1}{C}H_2-OH$

P-83.2.2 Names of selectively labeled compounds

The name of a selectively labeled compound is formed in the same way as the name of a specifically labeled compound, except that the multiplying subscripts following the atomic symbols are generally omitted. Identical locants corresponding to the same element are not repeated. The name of a selectively labeled compound differs from the name of the corresponding isotopically substituted compound in the use of square brackets, [ ], surrounding the nuclide descriptor rather than parentheses and in the omission of repeated identical locants and multiplying subscripts.

Examples:

Mixture of isotopically substituted compounds	**when added to**	**is named**
$CH_3{}^2H$, $CH_2{}^2H_2$ $CH{}^2H_3$, C^2H_4	CH_4	[^{2}H]methane (PIN) (not [$^2H_4$]methane)
$\overset{2}{C}H_2{}^2H-\overset{1}{C}H_2-OH$ $\overset{2}{C}H{}^2H_2-\overset{1}{C}H_2-OH$	CH_3-CH_2-OH	[1-^{2}H]ethan-1-ol (PIN) (not [1,1-$^2H_2$]ethan-1-ol)
${}^{14}\overset{3}{C}H_3-\overset{2}{C}H_2-\overset{1}{C}OO-CH_2-CH_3$ $\overset{3}{C}H_3-\overset{2}{C}H_2-\overset{1}{C}OO-{}^{14}CH_2-CH_3$	$CH_3-CH_2-COO-CH_2-CH_3$	[1-^{14}C]ethyl [3-^{14}C]propanoate (PIN)
$\overset{2}{C}H_2{}^2H-\overset{1}{C}H_2-OH$ $\overset{2}{C}H{}^2H_2-\overset{1}{C}H_2-OH$	CH_3-CH_2-OH	[2-$^2H_{1;2}$]ethan-1-ol (PIN)
$\overset{2}{C}H{}^2H_2-\overset{1}{C}H_2-OH$ $\overset{2}{C}H{}^2H_2-\overset{1}{C}H_2-{}^{18}OH$	CH_3-CH_2-OH	[2-$^2H_{2;2}$]ethan-1-[$^{18}O_{0;1}$]ol (PIN)

P-83.3 NONSELECTIVELY LABELED COMPOUNDS

P-83.3.1 An isotopically labeled compound is designated as nonselectively labeled when the position(s) and the number of the labeling nuclide(s) are both undefined.

When only atoms of an element to be modified are present at the same position in a compound, only specific or selective labeling can result. Nonselective labeling requires that the element to be modified be at different positions in the structure. For example, CH_4 and $CCl_3-CH_2-CCl_3$ can only be specifically or selectively labeled with a hydrogen isotope.

P-83.3.2 Structures

Nonselective labeling is indicated in a formula by inserting the nuclide symbol, enclosed in brackets, directly before the line formula without locants or subscripts.

Example:

[^{13}C]$CH_3-CH_2-CH_2-COOH$

P-83.3.3 Names

The name of a nonselectively labeled compound is formed in the same way as the name of a selectively labeled compound but contains neither locants nor subscripts in the nuclide descriptor.

Examples:

chloro[^{2}H]benzene (PIN)

[^{13}C]propane-1,2,3-triol (PIN)

[^{13}C]glycerol

P-83.4 ISOTOPICALLY DEFICIENT COMPOUNDS

P-83.4.1 An isotopically labeled compound may be designated as isotopically deficient when the isotopic content of one or more elements has (have) been depleted, i.e. when one or more nuclide(s) is(are) present in less than the natural ratio.

P-83.4.2 Structures

Isotope deficiency is denoted in the formula by adding the italicized symbol '*def*' immediately preceding, and without a hyphen, the appropriate nuclide symbol.

Example:

$[\textit{def}^{13}\text{C}]\text{CHCl}_3$

P-83.4.3 Names

The name of an isotopically deficient compound is formed by adding the italicized symbol *def* immediately preceding, and without a hyphen, the appropriate nuclide symbol, both enclosed in brackets and cited before the name or the part of the name that is isotopically modified.

Example:

trichloro[*def*^{13}C]methane (PIN)

[*def*^{13}C]chloroform

P-83.5 GENERAL AND UNIFORM LABELING

P-83.5.1 In the name of a selectively labeled compound in which all positions of the designated element are labeled, but not necessarily in the same isotopic ratio, the symbol ‘G’ is used in place of locants to indicate a ‘general’ labeling.

Examples:

Isotopically substituted compounds	**when added to**	**is designated as**
mixture of substituted compounds (selective labeling) CH_3-CH_2-CH_2-$^{14}COOH$ CH_3-CH_2-$^{14}CH_2$-$COOH$ CH_3-$^{14}CH_2$-CH_2-$COOH$ $^{14}CH_3$-CH_2-CH_2-$^{14}COOH$ etc.	CH_3-CH_2-CH_2-$COOH$	[G-^{14}C]butanoic acid (PIN)

D-Glucose in which all six positions are labeled with ^{14}C, but not necessarily uniformly, is designated as D-[G-^{14}C]glucose.

P-83.5.2 In the name of a selectively labeled compound in which all positions of the designated element are labeled in the same isotopic ratio, the symbol ‘U’ is used in place of locants to denote ‘uniform’ labeling.

Examples:

Isotopically substituted compounds	**when added to**	**is designated as**
mixture of substituted compounds (uniform labeling) CH_3-CH_2-CH_2-$^{14}COOH$ CH_3-CH_2-$^{14}CH_2$-$COOH$ CH_3-$^{14}CH_2$-CH_2-$COOH$ $^{14}CH_3$-CH_2-CH_2-$COOH$ in equal amounts	CH_3-CH_2-CH_2-$COOH$	[U-^{14}C]butanoic acid (PIN)

D-Glucose in which ^{14}C is equally distributed among the six positions is designated as D-[U-^{14}C]glucose.

Note: In the case of radioactive nuclides, ‘same isotopic ratio’ means ‘same specific radioactivity’.

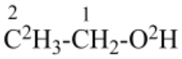
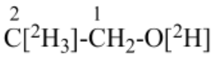
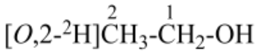
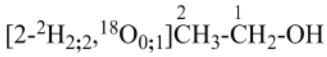
P-83.5.3 In the name of a selectively labeled compound, the symbol ‘U’ (see P-83.5.2) followed by appropriate locants is similarly used to indicate labeling in the same isotopic ratio at the specified positions.

Example:

D-glucose in which ^{14}C is equally distributed among positions 1, 3, and 5 is designated as D-[U-1,3,5-^{14}C]glucose.

P-84 COMPARATIVE EXAMPLES OF FORMULAS AND NAMES OF ISOTOPICALLY MODIFIED COMPOUNDS

Types of compounds	**Formula**	**Name**

Unmodified	CH_3-CH_2-OH	ethanol (PIN)
Isotopically substituted	 $\overset{2}{C}{}^{2}H_3\text{-}\overset{1}{C}H_2\text{-}O{}^{2}H$	(2,2,2-$^{2}H_3$)ethan-1-(^{2}H)ol (PIN) (*O*,2,2,2-$^{2}H_4$)ethan-1-ol
Specifically labeled	 $\overset{2}{C}[{}^{2}H_3]\text{-}\overset{1}{C}H_2\text{-}O[{}^{2}H]$	[2,2,2-$^{2}H_3$]ethan-1-[^{2}H]ol (PIN) [*O*,2,2,2-$^{2}H_4$]ethan-1-ol
Selectively labeled	 $[O,2\text{-}{}^{2}H]\overset{2}{C}H_3\text{-}\overset{1}{C}H_2\text{-}OH$	[2-^{2}H]ethan-1-[^{2}H]ol (PIN)
	 $[2\text{-}{}^{2}H_{2;2},{}^{18}O_{0;1}]\overset{2}{C}H_3\text{-}\overset{1}{C}H_2\text{-}OH$	[2-$^{2}H_{2;2}$]ethan-1-[$^{18}O_{0;1}$]ol (PIN)
Nonselectively labeled	[^{2}H]CH_3-CH_2-OH	[^{2}H]ethanol (PIN)
Isotopically deficient	[*def*^{13}C]CH_3-CH_2-OH	[*def*^{13}C]ethanol (PIN)

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Chapter P-9 SPECIFICATION OF CONFIGURATION AND CONFORMATION

- P-90 Introduction
- P-91 Stereoisomer graphical representation and naming
- P-92 The Cahn-Ingold-Prelog (CIP) priority system and the Sequence Rules
- P-93 Configuration specification
- P-94 Conformation and conformational stereodescriptors

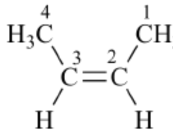
P-90 INTRODUCTION

This Chapter is concerned only with the main principles for specification of configuration and conformation of organic compounds. The structure of an organic compound is systematically indicated by one or more affixes added to a name that does not itself prescribe stereochemical configuration or conformation; such affixes are generally called ‘stereodescriptors’. Thus, stereoisomers, such as enantiomers, have names that differ only in the stereodescriptors used. In contrast, ‘*cis/trans*’ isomers may have different names because of different stereodescriptors or names differing in the type of nomenclature. Also, certain retained names imply their own stereochemical description, for example, maleic acid, cholesterol, and other natural products described in Chapter P-10.

In order to arrive at an unambiguous description of stereoisomers, Cahn, Ingold, and Prelog (refs. 34, 35) recommended an order of seniority for the ligands (atoms and groups) attached to carbon and other atoms, which is commonly called the ‘CIP priority system’. The priority is established by the application of ‘Sequence Rules’. These rules are discussed in P-92. Their application is then described for stereogenic units, mainly for the most usual compounds encountered in organic chemistry. Synthetic compounds are discussed in P-93 and Natural Products in Chapter P-10.

When different stereodescriptors are recommended to describe *cis* and *trans* isomers, diastereoisomers, and enantiomers, one of them is recommended as a preferred stereodescriptor. This preferred stereodescriptor is used to generate a preferred IUPAC name. Obviously, in general nomenclature, any appropriate descriptor can be used.

Example:



(2*Z*)-but-2-ene (PIN)
cis-but-2-ene

P-91 STEREOISOMER GRAPHICAL REPRESENTATION AND NAMING

- P-91.1 Stereoisomer graphical representation
- P-91.2 Stereodescriptors
- P-91.3 Naming of stereoisomers

P-91.1 STEREOISOMER GRAPHICAL REPRESENTATION

Structural diagrams which depict configurations must be prepared with extra care. Recommendations were made in 1996 to achieve that goal (ref. 37). A new set of recommendations is now proposed in the document entitled ‘Graphical representation of stereochemical configuration, IUPAC Recommendations 2006’ (ref. 38).

In general, plain lines depict bonds approximately in the plane of the drawing. Bonds to atoms above the plane are shown by a solid wedge ◀(starting from an atom in the plane of the drawing at the narrow end of the wedge); bonds to atoms below the plane are shown by a hashed wedge ┆┆┆┆interpreted in a sense similar to the solid wedge (starting from an atom in the plane of the drawing at the narrow end of the wedge). If the configuration is unknown, this can be indicated explicitly by a wavy line of constant amplitude 〰. These bonds are used in this book, with exceptions in the field of natural products clearly indicated in Chapter P-10 for carbohydrates.

In this Chapter, a single graphical representation depicts the absolute configuration of a chiral molecule.

P-91.2 STERODESCRIPTORS

The configuration of an organic compound is systematically indicated by one or more affixes added to a name that does not itself prescribe configuration; such affixes are called ‘stereodescriptors’.

P-91.2.1 Recommended stereodescriptors
P-91.2.2 Omission of stereodescriptors

P-91.2.1 Recommended stereodescriptors

Stereodescriptors are divided into two types:

P-91.2.1.1 Cahn-Ingold-Prelog (CIP) stereodescriptors
P-91.2.1.2 Other acceptable stereodescriptors

P-91.2.1.1 Cahn-Ingold-Prelog (CIP) stereodescriptors

Some stereodescriptors described in the Cahn-Ingold-Prelog (CIP) priority system, called ‘CIP stereodescriptors’, are recommended to specify the configuration of organic compounds, as described and exemplified in this Chapter and applied in Chapters P-1 through P-8, and in the nomenclature of natural products in Chapter P-10. The following stereodescriptors are used as preferred stereodescriptors (see P-92.1.2):

(a) ‘*R*’ and ‘*S*’, to designate the absolute configuration of tetracoordinate (quadriligant) chirality centers;

(b) ‘*r*’ and ‘*s*’, to designate the absolute configuration of pseudoasymmetric centers;

(c) ‘*M*’ and ‘*P*’, to specify the absolute configuration of an axial or planar entity using the helicity rule;

(d) ‘*m*’ and ‘*p*’, to specify the absolute configuration of a pseudoasymmetric entity using the helicity rule;

(e) ‘*seqCis*’ and ‘*seqTrans*’, to describe the configuration of enantiomorphic double bonds;

To specify the relative configuration the descriptor ‘*rel*’ associated with ‘*R*’ or ‘*S*’ is preferred to the stereodescriptors ‘*R**’ or ‘*S**’. Racemates are described by the descriptor ‘*rac*’ which is preferred to ‘*RS*’ or ‘*SR*’ stereodescriptors.

The following stereodescriptors are recommended for general nomenclature:

‘R_{a}’ and ‘S_{a}’ to specify the configuration of molecular entities possessing axial chirality;

‘R_{p}’ and ‘S_{p}’, to specify the configuration of molecular entities possessing planar chirality;

‘r_{a}’ and ‘s_{a}’, to specify the configuration of pseudoasymmetric stereogenic axes;

‘r_{p}’ and ‘s_{p}’, to specify the configuration of pseudoasymmetric stereogenic planes.

Capitalized CIP stereodescriptors are variant on reflection in a mirror (i.e. ‘*R*’ becomes ‘*S*’ and ‘*S*’ becomes ‘*R*’); lowercase CIP stereodescriptors are invariant on reflection in a mirror (i.e. ‘*r*’ remains ‘*r*’ and ‘*s*’ remains ‘*s*’). They are written in italics to indicate that they are not involved in the primary stage of alphanumerical order (see P-16.6).

P-91.2.1.2 Other acceptable stereodescriptors

Non Cahn-Ingold-Prelog (CIP) stereodescriptors are divided into two categories:

P-91.2.1.2.1 Stereodescriptors used in substitutive nomenclature;
P-91.2.1.2.2 Stereodescriptors used in the nomenclature of natural products (see Chapter P-10).

P-91.2.1.2.1 Stereodescriptors used in substitutive nomenclature

Stereodescriptors used in systematic substitutive names to specify the configuration of preferred IUPAC names and in general nomenclature; some stereodescriptors are recommended in general nomenclature only:

(a) Stereodescriptors used in preferred IUPAC names

(i) ‘*E*’ and ‘*Z*’ to describe the configuration of diastereomorphic alkenes $\mathrm{R^1R^2C{=}CR^3R^4}$ ($\mathrm{R^1 \neq R^2}$, $\mathrm{R^3 \neq R^4}$ and neither $\mathrm{R^1}$ nor $\mathrm{R^2}$ need be different from $\mathrm{R^3}$ or $\mathrm{R^4}$), cumulenes $\mathrm{R^1R^2C{=}[C{=}]_{\mathit{n}}CR^3R^4}$, systems for example, $\mathrm{R^1R^2C{=}NOH}$ and $\mathrm{HON{=}C\{[CH_2]_{\mathit{n}}\}_2C{=}NOH}$. The group of highest CIP priority attached to one of the terminal doubly bonded atoms of the alkene, oxime, etc., or cumulene (i.e. $\mathrm{R^1}$ or $\mathrm{R^2}$) is compared with the group of highest precedence attached to the other (i.e. $\mathrm{R^3}$ or $\mathrm{R^4}$). The stereoisomer is designated as ‘*Z*’ (zusammen = together) if the groups lie on the same side of a reference plane passing through the double bond and perpendicular to the plane containing the bonds linking the groups to the double bond atoms; the other isomer is designated ‘*E*’ (entgegen = opposite). The descriptors may be applied to structures with a fractional bond order between one or two; and to double bonds involving elements other than carbon.

(ii) '*A*' and '*C*' to describe the absolute configuration of pentacoordinate (pentaligant, as in a trigonal bipyramid or square pyramid) and hexacoordinate (hexaligant, as in an octahedron) stereogenic centers.

(b) The following stereodescriptors are recommended for general nomenclature:

(i) '*cis*', '*trans*' and '*r*', '*c*', '*t*' are used to specify the configuration of diastereomorphic double bonds (see P-93.4.2.1.1) and the relative configuration of alicyclic compounds (see P-93.5.1.3), respectively;

(ii) '*endo*', '*exo*', '*syn*', and '*anti*' are used to specify the relative configuration of some von Baeyer ring systems (see P-93.5.2.2.1).

In preferred IUPAC names, stereodescriptors, preceded by a locant, **must be** cited to specify each stereogenic unit, as illustrated in P-91.3. When the configuration is not known or must remain unspecified for lack of configurational homogeneity, the italicized symbol '*ξ*' or '*Ξ*' is used, preceded by the required locant (see P-91.3). The symbol 'ξ' (small Greek letter 'xi') replaces noncapitalized CIP stereodescriptors such as '*r*', '*s*', '*m*', '*p*'. The symbol 'Ξ' (capital Greek letter 'xi') replaces capitalized CIP stereodescriptors such as '*R*', '*S*', '*M*', '*P*', '*E*', '*Z*', '*seqCis*', and '*seqTrans*'.

P-91.2.1.2.2 Stereodescriptors used in the nomenclature of natural products (see Chapter P-10):

(i) The descriptors 'D' and 'L' are used to describe the configuration of carbohydrates (ref. 27 and P-102), amino acids and peptides (ref. 18 and P-103), and cyclitols (ref. 39 and P-104);

(ii) The descriptors '*erythro*' and '*threo*' are used in the systematic nomenclature of carbohydrates, along with descriptors such as '*arabino*' and '*gluco*' (see ref. 27 and P-102);

(iii) The stereodescriptors 'α', 'β' are used in the nomenclature of natural products to describe the absolute configuration of alkaloids, terpenes and terpenoids, steroids, and other compounds as described in P-101;

(iv) The stereodescriptors '*cis*', '*trans*' and '*all-E*' and '*all-trans*' are used in the nomenclature of carotenoids and similar compounds (see ref. 40 and P-101.6);

(v) The descriptor '*meso*' is used in the nomenclature of carbohydrates to designate compounds such as alditols and aldaric acids that are symmetrical and thus optically inactive (see P-102.5.6.5.2; P-102.5.6.6.5);

(vi) The stereodescriptor '*ambo*' describes the formation of diastereoisomers by reaction at a nonstereogenic center of a chiral molecule or the reaction of a chiral compound with a racemic compound which will not normally give a 50:50 mixture. To indicate this, the prefix '*ambo*' is used (see P-93.1.4 and P-103.3.4)

P-91.2.2 Omission of stereodescriptors

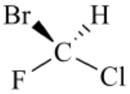
The omission of stereodescriptors specifying double bonds is recommended in the case of three- through seven-membered unsaturated alicyclic compounds where any double bond has a fixed configuration, '*Z*' in the case of hydrocarbons, and '*Z*' or '*E*' in accordance with the nature of ligands attached to the double bond (see P-93.5.1.4.1). Names such as 'cyclohexene' or 'cyclohepta-1,3,5-triene' are unambiguous; the addition of the stereodescriptor '*Z*' would add no further information. In eight-membered rings, the stereodescriptor '*Z*' or '*E*', with its locant, is required: in preferred IUPAC names when one double bond is present, i.e. in '(*Z*)-cyclooctene' and '(*E*)-cyclooctene', but not in the corresponding di-, tri-, or tetraene, i.e. 'cycloocta-1,3,5,7-tetraene'. From nine-membered rings onwards, stereodescriptors are required. The omission of stereodescriptors is also recommended in names of von Baeyer systems (P-93.5.2.3), spiro compounds (P-93.5.3.3), fused systems (P-93.5.4), cyclophane systems (P-93.5.5.3), and assemblies of identical rings and ring systems (P-93.5.7.3).

P-91.3 NAMING OF STEREOISOMERS

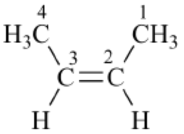
Stereodescriptors are added to a name constructed in accordance with the procedure of formation of preferred IUPAC names described in P-59.1. The rule expressed in Rule E-0 (ref. 1) and in R-7.0 (ref. 2) that 'stereodescriptors do not change the name or the numbering of a compound established by the principles, rules and conventions of nomenclature described in these recommendations' is still valid, especially for preferred IUPAC names. Nesting symbols may change the nesting pattern established before the introduction of these affixes. This issue is discussed and illustrated in P-16.5.4.1 and P-93.6.

In preferred IUPAC names, stereodescriptors are placed immediately at the front of the part of the name to which they relate. They are placed at the front of the complete name when related to the parent structure; they are cited in parentheses followed by a hyphen. When they relate to substituent groups, they are cited at the front of the corresponding prefix. They are preceded by a numerical or letter locant to describe the position of the stereogenic unit when such locants are present; general rules of numbering are applied (see P-14.4).

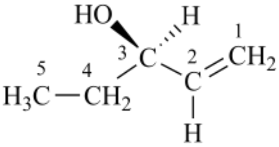
Examples:



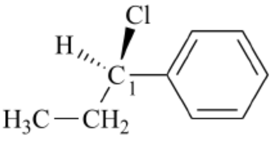
(*R*)-bromo(chloro)(fluoro)methane (PIN)



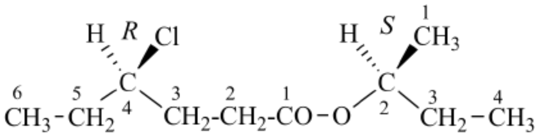
(2*Z*)-but-2-ene (PIN)



(3*R*)-pent-1-en-3-ol (PIN)
(see P-92.2.1.2)



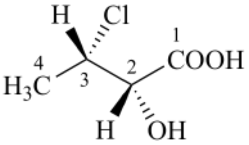
[(1*R*)-1-chloropropyl]benzene (PIN)



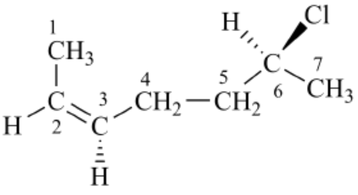
(2*S*)-butan-2-yl (4*R*)-4-chlorohexanoate (PIN)

When a molecule contains more than one stereogenic unit, the above mentioned procedure is applied to each sterogenic unit, and the configuration of the parent structure is expressed as a set of symbols. In names of compounds, the symbols, with their locants, are written in parentheses and separated by a comma, followed by a hyphen, at the front of the complete name or substituent. Multiple stereodescriptors are cited in the increasing order of their respective locants.

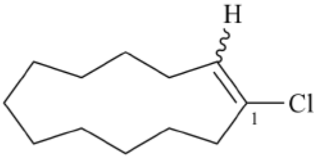
Examples:



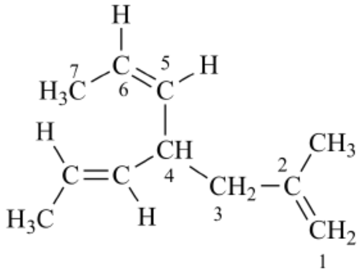
(2*S*,3*S*)-3-chloro-2-hydroxybutanoic acid (PIN)



(2*Z*,6*S*)-6-chlorohept-2-ene (PIN)
(for numbering, see P-14.4)



(1Ξ)-1-chlorocyclododec-1-ene (PIN)



(5*Z*)-4-[(1*E*)-prop-1-en-1-yl]hepta-1,5-diene (PIN)
Note: In illustrating just the double bonds, the stereodescriptor of the chirality center at ‘C-4’ is not included in the name.

P-92 THE CAHN-INGOLD-PRELOG (CIP) PRIORITY SYSTEM AND THE SEQUENCE RULES

P-92.1 The Cahn-Ingold-Prelog (CIP) System: General methodology
P-92.2 Sequence Rule **1**
P-92.3 Sequence Rule **2**
P-92.4 Sequence Rule **3**
P-92.5 Sequence Rule **4**
P-92.6 Sequence Rule **5**

P-92.1 THE CAHN-INGOLD-PRELOG (CIP) SYSTEM: GENERAL METHODOLOGY

P-92.1.1 Stereogenic units
P-92.1.2 Rules for the assignment of configuration
P-92.1.3 The Sequence Rules
P-92.1.4 Hierarchical digraphs
P-92.1.5 Exploration of a hierarchical digraph
P-92.1.6 Ligand ranking: application of the five Sequence Rules

P-92.1.1 Stereogenic units

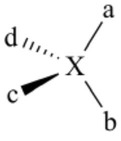
A stereogenic unit (i.e. a unit generating stereoisomerism) is a grouping within a molecular entity that may be considered to generate stereoisomerism. At least one stereogenic unit must be present in every chiral molecule; however, conversely, the presence of stereogenic units does not require the corresponding molecular entity to be chiral. In preferred IUPAC names, all stereogenic units must be specified, unless an omission is allowed according to P-91.2.2.

Chirality is the property of an object, thus of a molecular entity, of being nonsuperposable on its mirror image. If the object (molecular entity) is superposable on its mirror image, it is said to be ‘achiral’. Usual configurational terms used in this Chapter are defined in ref. 37.

The basic types of stereogenic units in molecular entities involving atoms having not more than four ligands are considered below:

(a) A chirality center. A grouping of atoms consisting of a central atom ‘X’ and distinguishable ligands ‘a’,‘b’, ‘c’, ‘d’, so that the interchange of any two of the ligands ‘a’, ‘b’, ‘c’, or ‘d’ leads to a stereoisomer (see also P-93.5.3.2).

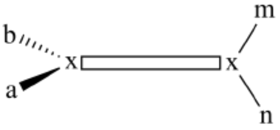
Example:



A chirality center denoted by ‘*R*’ for the sequence ‘a > b > c > d’

(b) A chirality axis. An axis about which a set of ligands is held so that it results in a spatial arrangement which is not superposable on its mirror image. For example, with an allene, ‘abC=C=Cmn’, the chirality axis is defined by the ‘C=C=C’ bonds; and with an *ortho*-substituted 1,1′-biphenyl the atoms ‘C-1’, ‘C-1″’, ‘C-4’, and ‘C-4″’ lie on the chirality axis (see ref. 37).

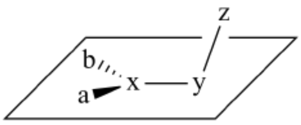
Example:



A chirality axis denoted by ‘*M*’ for the sequence‘a > b’ and ‘m > n’

(c) A chirality plane. A planar unit ‘a-x-b’ connected to an adjacent part of the structure by an out-of-plane bond ‘y-z’ which results in restricted torsion so that the plane cannot lie in a symmetry plane.

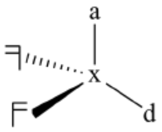
Example:



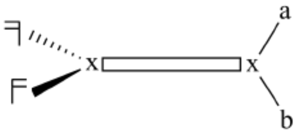
A chirality plane denoted by ‘*M*’ for ‘a > b’

(d) Stereogenic units are called pseudoasymmetric (center, axis or plane) when they have distinguishable ligands ‘a’, ‘b’, ‘c’, ‘d’, two and only two of which are nonsuperposable mirror images of each other (enantiomorphic). These enantiomorphic ligands are represented by ‘ ╒ and ╕ ’ as designated by Prelog and Helmchen (see ref. 36). The ‘*r/s*’ and ‘*m/p*’ stereodescriptors describing a pseudoasymmetric stereogenic unit are invariant on reflection in a mirror (for example ‘*r*’ remains ‘*r*’, and ‘*s*’ remains ‘*s*’), but are reversed by the exchange of any two ligands (‘*r*’ becomes ‘*s*’, and ‘*s*’ becomes ‘*r*’). Lower case stereodescriptors are used to describe pseudoasymmetric stereogenic units.

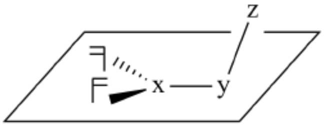
Examples:



A pseudoasymmetric stereogenic unit denoted by ‘*r*’ for ‘a > ╒ > ╕ > d’
(‘ ╒ ’ and ‘ ╕ ’ are enantiomorphic ligands)



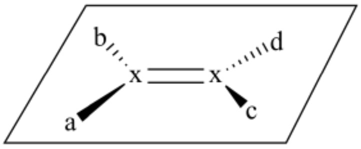
A pseudoasymmetric stereogenic unit denoted by ‘*m*’ for ‘a > b and ╒ > ╕ ’
(‘ ╒’ and ‘╕ ’ are enantiomorphic ligands)



A pseudoasymmetric stereogenic unit denoted by ‘*m*’ for ‘ ╒ > ╕ ’
(‘ ╒ ’ and ‘ ╕ ’ are enantiomorphic ligands)

(e) *cis/trans* Isomers containing a double bond. A grouping of atoms consisting of a double bond with different ligands which give rise to *cis-trans* isomerism.

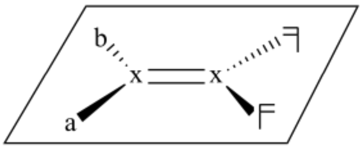
Example:



A double bond denoted as ‘*E*’ for ‘a > b’ and ‘d > c’

(f) An enantiomorphic double bond

Example:



An enantiomorphic double bond denoted *seqCis* for ‘a > b’ and ‘ ╒ > ╕ ’
(‘ ╒’ and ‘╕ ’ are enantiomorphic ligands)

P-92.1.2 Rules for the assignment of configuration

This section describes the CIP priority system which was developed to deal with all compounds with a bonding number up to six for organic compounds, and for all configurations and conformations of these compounds (refs. 34, 35, 36). Its description for specifying configurations and conformations is discussed herein.

P-92.1.2.1 The chirality rule and the stereodescriptors ‘*R*’, ‘*S*’, ‘R_a’, ‘S_a’, ‘R_p’, ‘S_p’

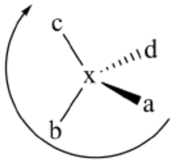
For a tetrahedral stereogenic unit having four different ligands, the chirality rule is based on the arrangement of these ligands (including chains and rings) in an order of precedence, often referred to as an order of priority. For discussion this order can conveniently be generalized as ‘a > b > c > d’, where ‘>’ means ‘has priority over’ or ‘has precedence over’. The order of precedence is reached by the construction of a hierarchical digraph and the application of the Sequence Rules as explained below.

The chirality rule is expressed by Prelog and Helmchen (see subsection 5.1, ref. 36) as follows: “Among ligands of highest precedence the path of their sequence is followed from the preferred side of the model, that is, the side remote from the group of lowest precedence, and, depending on whether the path turns to right or left, the chirality unit will be assigned the chiral label ‘*R*’ or ‘*S*’, or, if pseudoasymmetric, ‘*r*’ or ‘*s*’”.

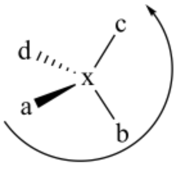
This rule is applied to stereogenic centers, stereogenic axes, and stereogenic planes.

P-92.1.2.1.1 Stereogenic centers

For ‘a > b > c > d’, two enantiomeric stereogenic centers are described as ‘*R*’ or ‘*S*’ depending of the sense of chirality as shown below.



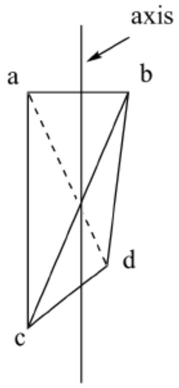
R



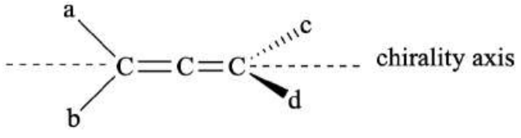
S

P-92.1.2.1.2 Stereogenic axes

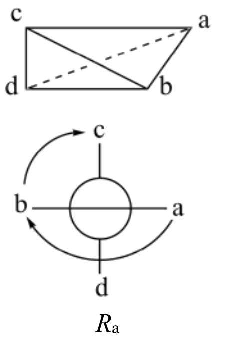
Structures with axial chirality are regarded as elongated tetrahedra and viewed along the axis; it is immaterial from which side they are viewed (see subsection 2.5.2, ref. 36). Axial chirality is used to refer to stereoisomerism resulting from the nonplanar arrangement of four groups in pairs about a chirality axis. A chirality axis is the axis about which a set of atoms or groups is held so that a spatial arrangement results which is not superposable on its mirror image. For instance, in an allene ‘abC=C=Ccd’, the chirality axis is defined by the ‘C=C=C’ bonds, and in a ‘2,2′,6,6″-tetrasubstituted 1,1′-biphenyl the atoms ‘1,1′,4,4″’ lie on the chirality axis.



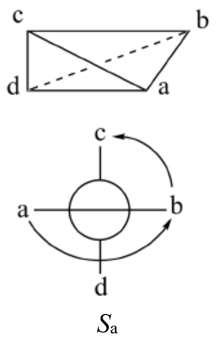
In chiral compounds owing their chirality to a stereogenic center, it is necessary to have four different atoms or groups ‘a’, ‘b’, ‘c’, and ‘d’. With an elongated tetrahedron, this requirement is no longer necessary because of reduced symmetry. The only condition is that ‘a’ be different from ‘b’, and ‘c’ be different from ‘d’; thus compounds with two pairs of ligands ‘a’ and ‘b’ are chiral if ‘a’ is different than ‘b’.



The configuration is specified by the descriptors ‘R_a’ and ‘S_a’ assigned as follows:



R_a

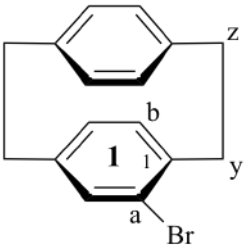


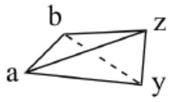
S_a

Ligands (atoms or groups) are arranged in the elongated tetrahedral system. Two higher-ranking substituents are chosen, one in each pair, using the Sequence Rule. For the pairs ‘a > b’ and ‘c > d’, the chirality is described by the symbol ‘R_a’ if the path going from ‘a to b to c’ is clockwise, while looking toward ‘d’. The chirality symbol is ‘S_a’ if this path is anticlockwise.

P-92.1.2.1.3 Stereogenic planes

Planar chirality is a term used to refer to stereoisomerism resulting from the arrangement of out of plane groups with respect to a plane (stereogenic plane) (see 2.5.2, ref. 36). It is exemplified by the atropisomerism of a monosubstituted cyclophane in which the stereogenic plane is the substituted ‘phane amplificant’ (see P-26). The configuration is specified by the stereodescriptors ‘R_p’ and ‘S_p’ assigned as follows:





A tetrahedron (tetrahedral stereogenic unit) is derived by connecting the in-plane reference atoms ‘a’ and ‘b’ to the atoms ‘y’ and ‘z’. The chirality sense is determined by conventional rules establishing the priority order ‘a > b > c > d’ or ‘a > b > y > z’ for the cyclophane above. Thus, the descriptor ‘S_p’ is used to denote the configuration and assigned to the carbon atom ‘C-1^1’.

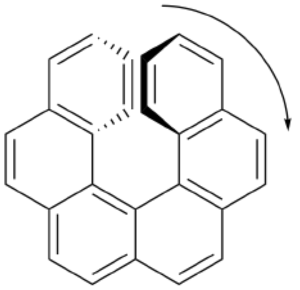
P-92.1.2.2 The helicity rule: stereodescriptors ‘*M*’ and ‘*P*’

Helicity is the chiral sense of a helical, propeller, or screw-shaped molecular entity (see ref. 37). The ‘helicity’rule is expressed by Prelog and Helmchen (see subsection 5.1, ref. 36) as: “Depending on whether the identified helix is left- or right-handed, it is designated ‘minus’ and marked ‘*M*’ or ‘plus’ and marked ‘*P*’ ”.

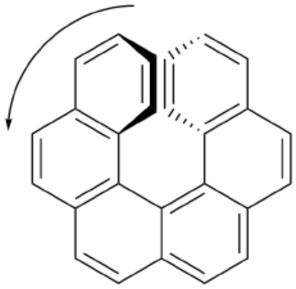
The application of this system to the description of conformations and configurations considers the torsion angle between two reference groups attached to the atoms at each end of a bond or an axis. The sign of the smaller torsion angle between the reference groups defines the chirality sense of the corresponding stereogenic unit (see torsion angle, P-94.2).

P-92.1.2.2.1 Stereogenic axis

The chirality of hexahelicenes is denoted by the stereodescriptors ‘*P*’ and ‘*M*’.

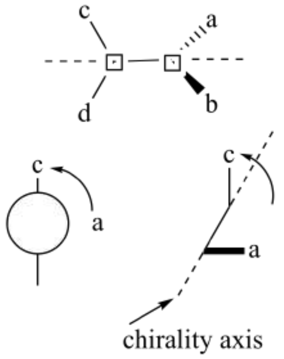


(*P*)-hexahelicene (PIN)

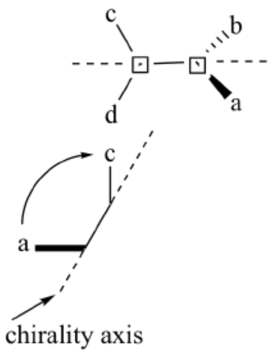


(*M*)-hexahelicene (PIN)

The helicity rule can also be applied to the stereogenic axis in allenes and biphenyls. Looking along the chirality axis the ligands are arranged in pairs. When proceeding from the nearer ligand having priority in the pair to the further away atom or group having priority in the pair, the chirality is described by the symbols ‘*M*’ if the path is anticlockwise; the symbol is ‘*P*’ if the path is clockwise. Stereodescriptors ‘*M*’ and ‘*P*’ are used in preferred IUPAC names. The lowest locant on the axis is cited before the stereodescriptor.



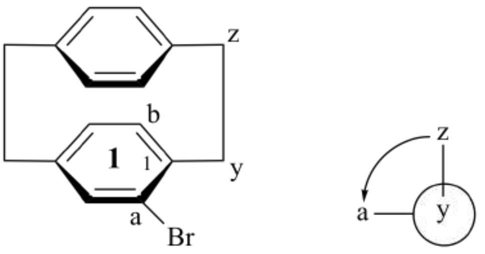
M



P

P-92.1.2.2.2 Stereogenic plane

Stereodescriptors '*M*' and '*P*' are assigned as follows:



M

The reference plane of the molecule is described by 'a > b'. The out-of-plane component is described by 'z', attached to the in-plane axis 'x-y'. A negative torsion angle is denoted when 'z' is rotated into the plane in the direction of 'a' that has precedence over 'b'. The stereodescriptor '*M*' is used to denote the configuration shown above. The lowest locant in the reference plane is cited before the stereodescriptor.

P-92.1.2.2.3 There is no general correspondence between '*R/S*' and '*M/P*' descriptors. In fact, using the conventions described above for the specification of the configuration, for a chirality axis '*M*' = '*R*' and '*P*' = '*S*'; for chirality planes the opposite relationship is to be noted where '*M*' = '*S*' and '*P*' = '*R*'.

P-92.1.3 The 'Sequence Rules'

The following 'Sequence Rules' are used (refs 34, 35, 36) to establish the order of precedence of atoms and groups. A more encompassing set of rules, proposed by Mata, Lobo, Marshall, and Johnson (ref. 41), including amendments by Custer (ref. 42) and Hirschmann and Hanson (ref. 43), is used in this Chapter.

These rules are based on the hierarchical order of ligands properties, material, and topological properties for the Sequence Rules **1** and **2**, geometrical properties for Sequence Rules **3** and **4**, and topographical properties for Sequence Rule **5**. Properties associated with the first four Sequence Rules are reflection-invariant, while that associated with the fifth is reflection-variant.

Ligands are monodentate (monovalent, acyclic) or *n*-dentate (cyclic) as exemplified in P-92.2.1.3.

The Sequence Rules are hierarchical, i.e., each rule must be exhaustively applied in the order given until a decision is reached:

P-92.1.3.1 Sequence Rule **1** has two parts:

(a) higher atomic number precedes lower;

(b) a duplicate atom node whose corresponding nonduplicated atom node is the root or is closer to the root ranks higher than a duplicate atom node whose corresponding nonduplicated atom node is farther from the root.

P-92.1.3.2 Sequence Rule **2**

Higher atomic mass number precedes lower;

P-92.1.3.3 Sequence Rule **3**

When considering double bonds and planar tetraligand atoms '*seqcis*' = '*Z*' precedes '*seqtrans*' = '*E*' and this precedes nonstereogenic double bonds.

P-92.1.3.4 Sequence Rule **4** is best considered in three parts

(a) Chiral stereogenic units precede pseudoasymmetric stereogenic units and these precede nonstereogenic units.

(b) When two ligands have different descriptor pairs, then the one with the first chosen *like* descriptor pairs has priority over the one with a corresponding *unlike* descriptor pair (see P-92.5.2.1 for a discussion and examples about this rule).

(i) *like* descriptor pairs are: '*R-R*', '*S-S* ', '*M-M* ', '*P-P* ', '*R-M*', '*S-P*', '*seqCis-seqCis*', '*seqTrans-seqTrans*', '*R-seqCis*', '*S-seqTrans*', '*M-seqCis*', '*P-seqTrans*'...;

(ii) *unlike* descriptor pairs are '*R-S*', '*M-P*', '*R-P*', '*S-M*', '*seqCis-seqTrans*', '*R-seqTrans*', '*S-seqCis*', '*P-seqCis*', '*M-seqTrans*'....

(c) '*r*' precedes '*s*' and '*m*' precedes '*p*'

P-92.1.3.5 Sequence Rule **5**

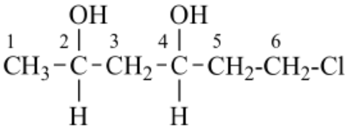
An atom or group with descriptor '*R*', '*M*', and '*seqCis*' has priority over its enantiomorph '*S*', '*P*' or '*seqTrans*'.

P-92.1.4 Hierarchical digraphs

In order to establish the order of precedence of ligands in a stereogenic unit, the atoms of the stereogenic unit are rearranged in a hierarchical diagram, called a 'digraph' or 'tree-graph', representing the connectivity (topology) and make-up of atoms; a digraph originates from the core of the stereogenic unit and is developed by indicating the various branches (see section 3, ref. 36) representing ligands. A digraph must be established for each stereogenic unit generating several digraphs when several stereogenic units are present in a molecule. Each skeletal atom of the molecule is numbered, either by using the systematic numbering recommended in the nomenclature of organic compounds or by using an arbitrary numbering for the sole purpose of ranking ligands as described in P-92.1.6. Specific rules apply to acyclic molecules, double and triple bonds, and cyclic molecules.

P-92.1.4.1 Acyclic molecules

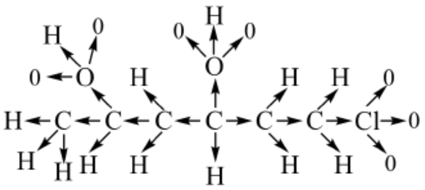
The digraphs corresponding to 6-chlorohexane-2,4-diol are illustrated.



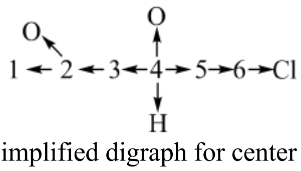
$CH_3\text{-}CH(OH)\text{-}CH_2\text{-}CH(OH)\text{-}CH_2\text{-}CH_2\text{-}Cl$

6-chlorohexane-2,4-diol (PIN)

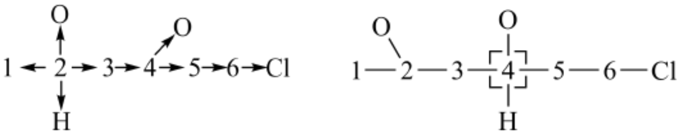
The complete digraph describes all monodentate ligands; to ensure the tetraligancy of all atoms, except H, 'phantom atoms' are shown. These atoms have the atomic number zero shown by the symbol '0'. Such complete digraphs are useful in complex cases, but most of the time for simple compounds simplified digraphs are satisfactory; they show the relevant information necessary to rank ligands. Two types of simplified digraphs are shown in which symbols of skeletal atoms are replaced by locants used to describe the molecule; hydrogen atoms and phantom atoms are omitted. The third and fifth ones, without arrows, will be used throughout this Chapter, with a clear indication, however, of the stereogenic unit that is described.



the complete digraph for center 4



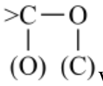
simplified digraph for center 4

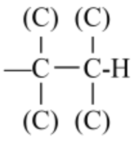
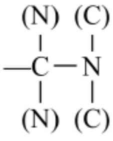


simplified digraph for center 2

P-92.1.4.2 Double and triple bonds

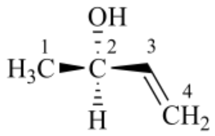
Using the Sequence Rules depends on exploring along bonds. To avoid theoretical arguments about the nature of bonds, some classical forms are used. Double and triple bonds are split into two or three bonds respectively.

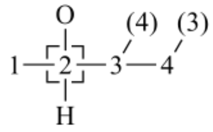
A >C=O group is treated as  where (O) and (C) are duplicate representations of the atoms at the other end of the double bond.

Similarly, a –C≡CH group is treated as  where (C) is a duplicate representations of the atoms at the other end of the triple bond and a –C≡N group is treated as  where (C) and (N) are duplicate representations of the atoms at the other end of the triple bond.

Only the doubly bonded atoms themselves are duplicated, and not the atoms or groups attached to them; the duplicated atoms may thus be considered as carrying three phantom atoms (see above) of atomic number zero. This may be important in deciding priorities in more complicated cases.

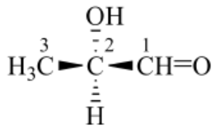
The simplified digraph corresponding to the ethylenic alcohol ‘but-3-en-2-ol (PIN)’ is as follows:

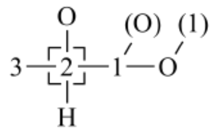




simplified digraph showing duplicate atoms

The digraph corresponding to ‘2-hydroxypropanal (PIN)’ is as follows:



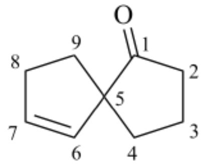


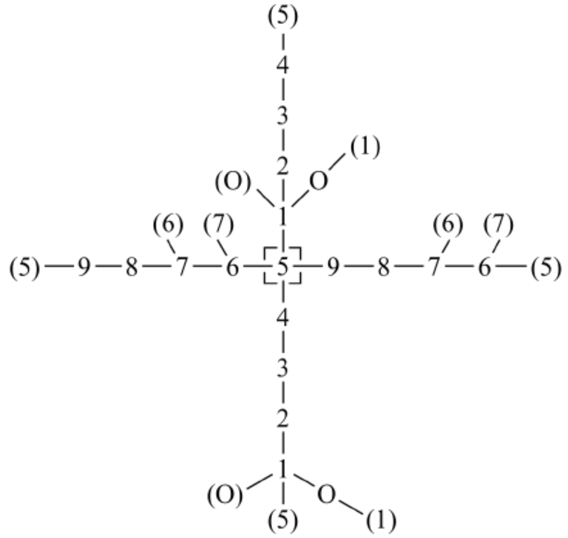
simplified digraph showing duplicate atoms

P-92.1.4.3 Saturated rings and ring systems

The methodology to transform the constitutional formula of a cyclic molecule into an acyclic digraph has been recommended by Prelog and Helmchen (see subsection 3.2, ref. 36).

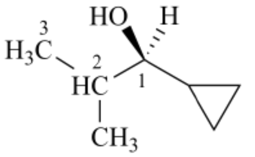
In order to obtain the acyclic digraph of a stereogenic unit the *n*-dentate ligand is transformed into *n* monodentate ligands, by leaving intact in each case one bond with the core and cleaving the *n*−1 bonds. At each end of *n* branches thus obtained a duplicate atom of the core is attached (as in the case of multiple bonds described in P-92.1.4.2).



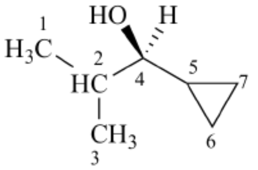


simplified digraph for center 5

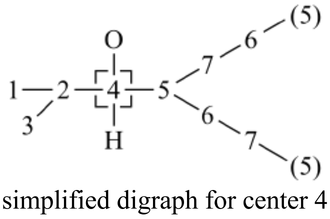
In ligands of stereogenic units containing rings, the ring opens after the first ring atom encountered when exploring each way outward from the core; one bond remains intact while the other is cleaved. A duplicate of the first encountered ring atom is attached at the end of the two branches thus obtained.



(1*R*)-1-cyclopropyl-2-methylpropan-1-ol (PIN)



numbering for the simplified digraph

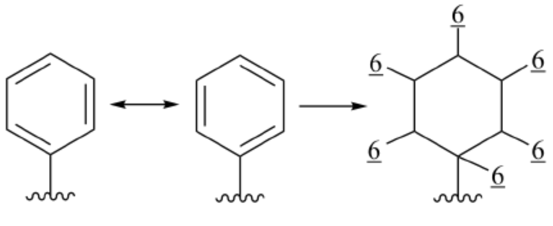


simplified digraph for center 4

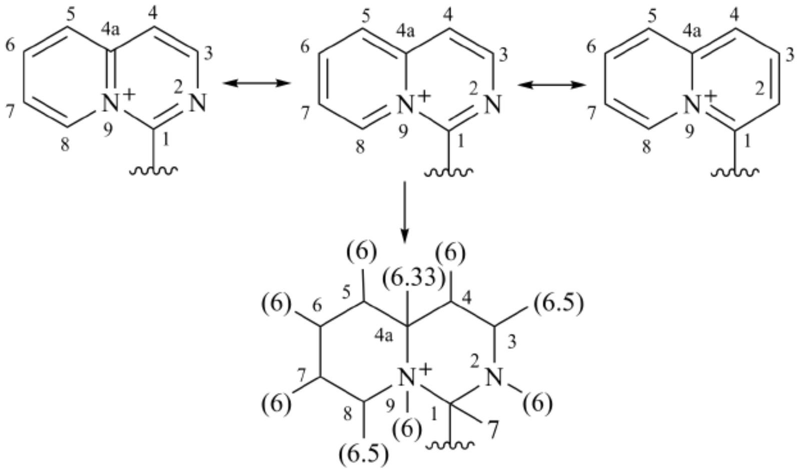
P-92.1.4.4 Mancude rings and ring systems

Mancude rings, i.e., rings or ring systems having the maximum number of noncumulative double bonds, are treated as Kekulé structures. For mancude heterocycles, each duplicate atom is given an atomic number that is the mean of what it would have if the double bonds were located at each of the possible positions. For mancude hydrocarbons, it is immaterial which Kekulé structure is used because 'splitting' the double bonds gives the same result in all cases.

The atomic number 6 is always present, as exemplified for a phenyl group:

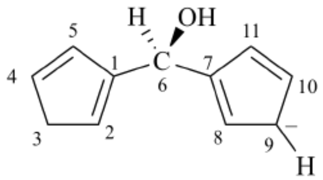


And for an example involving nitrogen atoms

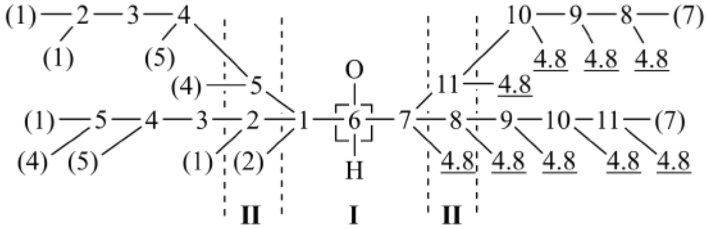


Explanation: ‘C-1’ is doubly bonded to one or the other of the nitrogen atoms and never to carbon, so its added duplicate atom has an atomic number of 7 (that of nitrogen). ‘C-3’ is doubly bonded either to ‘C-4’ (atomic number 6) and to ‘N-2’ (atomic number 7); so its added duplicate atom has an atomic number of 6½, as it is for ‘C-8’. But ‘C-4a’ may be doubly bonded to ‘C-4’, ‘C-5’ and ‘N-9’, so its added duplicate atom has an atomic number of 6⅓.

Example:



3-[(*S*)-(cyclopenta-1,4-dien-1-yl)(hydroxy)methyl]cyclopenta-2,4-dien-1-ide (PIN)



simplfied digraph showing seniority of branch ‘C-1’ over ‘C- 7’,
because the atomic numbers 6 for ‘C-2’ > ‘4.8’ in sphere **II**,
thus leading to an ‘*S*’ configuration for ‘C-6’.

Explanation: Five different Kekulé structures should be considered for the right hand ligand for each carbon atom in the ring. For four of them they are doubly bonded to another carbon atom; for the fifth atom the electron pair with atomic number ‘zero’ must be taken into consideration. Thus 4 x 6 + 0 = 24; 24/5 = 4.8, that is the atomic number for each carbon atom in the right ligand.

P-92.1.5 Exploration of a hierarchical digraph

Digraphs are constructed to show the ranking of atoms according to the topological distance i.e., number of bonds, from the core of the stereogenic unit (i.e., center) and their evaluation by the Sequence Rules (see subsection 3.2, ref. 36).

(a) Atoms lie in spheres and atoms of equal distance from the core of the stereogenic unit are in the same sphere; spheres are identified as **I**, **II**, **III**, and **IV**, as shown in **Fig. 9.1**. The first sphere is occupied by the ‘proximal atoms’, ‘p’ and ‘p′’. Those in the sphere **II** are numbered ‘1,2,3’ and ‘1′,2′,3′’. Those in sphere **III** are numbered ‘11’, ‘12’, ‘13’, ‘21’, ‘22’, ‘23’,... ‘11′’, ‘12′’, ‘13′’... and so on for each further sphere. Indicated branches may not be present in all molecules.

(b) Atoms in the *n*th sphere have precedence over those in the $(n + 1)$th sphere (Ranking Rule **1**).

(c) The ranking of each atom in the *n*th sphere depends in the first place on the ranking of atoms of the same branch in $(n - 1)$th sphere, and then the application of the Sequence Rules to it; the smaller the number, the higher the relative ranking (Ranking Rule **2**).

(d) Those atoms in the *n*th sphere which are of equal rank with respect to those in the $(n - 1)$th sphere in the same branch are ranked by means of the Sequence Rules, first by the exhaustive application of Sequence Rule **1**; if no decision is reached, Sequence Rule **2** is exhaustively applied, and so on.

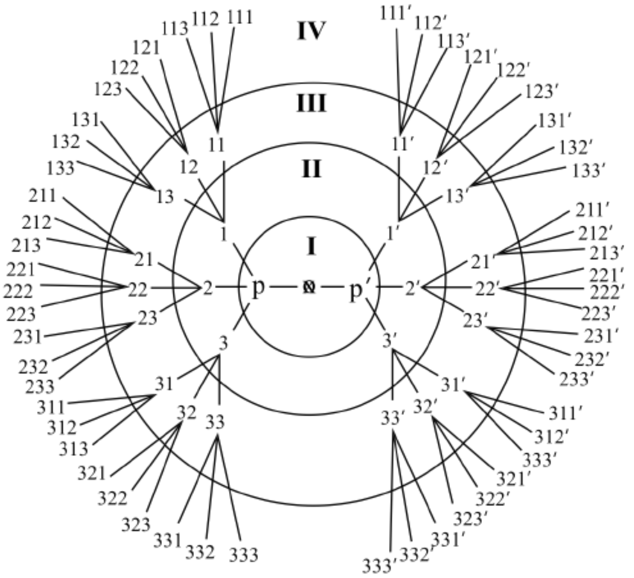

IV
III
II
I
p
p′
1
2
3
1′
2′
3′
11
12
13
21
22
23
31
32
33
11′
12′
13′
21′
22′
23′
31′
32′
33′
111 112 113 121 122 123 131 132 133
211 212 213 221 222 223 231 232 233
311 312 313 321 322 323 331 332 333
111′ 112′ 113′ 121′ 122′ 123′ 131′ 132′ 133′
211′ 212′ 213′ 221′ 222′ 223′ 231′ 232′ 233′
311′ 312′ 333′ 321′ 322′ 323′ 331′ 332′ 333′

Fig. 9.1 Ranking order for two ligands

P-92.1.6 Ranking of ligands: Application of the Sequence Rules

The five ‘Sequence Rules’ discussed in P-92.1.3 are applied as follows:

(a) each rule is applied in accordance with a hierachical digraph (see P-92.1.4)

(b) each rule is applied exhaustively to all ligands being compared;

(c) the ligand that is found to have precedence (priority) at the first occurrence of a difference in a digraph retains this precedence (priority) regardless of differences that occur later in the exploration of the digraph;

(d) precedence (priority) of an atom in a group established by a rule does not change on application of a subsequent rule.

P-92.2 SEQUENCE RULE **1** (consisting of two subrules)

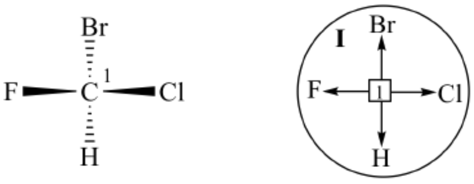
P-92.2.1 Sequence subrule **1a**: Ligands are arranged in order of decreasing atomic number.

In all examples shown below, ligands are ranked as ‘a > b > c > d’ for stereogenic units, unless otherwise stipulated for stereogenic axes and planes.

P-92.2.1.1 Saturated compounds

P-92.2.1.1.1 Sphere **I.**

Example 1:

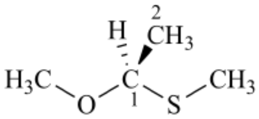

Br
F
C
1
Cl
H
I
Br
F
1
Cl
H

digraph for sphere **I**

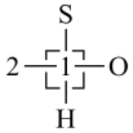
Explanation: In the compound HCBrClF, all atoms are included in sphere **I**. The order ‘a > b > c > d’ is ‘Br > Cl > F > H’ for center ‘1’ describing a clockwise direction; the stereodescriptor ‘*R*’ describes this configuration, leading to the preferred IUPAC name:

(*R*)-bromo(chloro)(fluoro)methane (PIN)

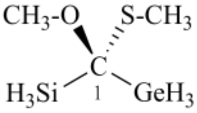
Example 2:

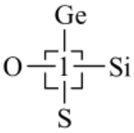

2
H
CH3
H3C
C
CH3
O
1
S

(1*R*)-1-methoxy-1-(methylsulfanyl)ethane (PIN)


simplified digraph for sphere **I**

Example 3:

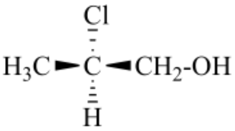

[(*R*)-germyl(methoxy)(methylsulfanyl)methyl]silane (PIN)
(the locant ‘1’ is related to the digraph; it is not required in the name)

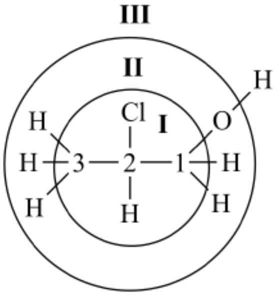

simplified digraph for sphere **I**

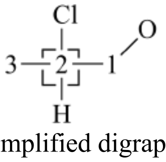
P-92.2.1.1.2 Spheres **I** and **II**

When atoms attached to the stereogenic unit are identical, precedence is established by the atoms in turn that are directly attached to the identical atoms. When the molecule contains several atoms and branches, it is convenient to number it, either by using the numbering system recommended in nomenclature or by applying an arbitrary system to properly identify all nodes appearing in the digraph.

Example 1:



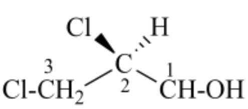

complete digraph for center 2

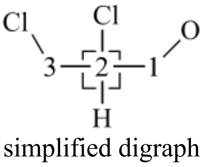

simplified digraph

Explanation: In the compound H_3C-CHCl-CH_2OH, above, the order of seniority for ‘a > b > c > d’ is ‘Cl > C = C > H’. No decision is reached in sphere **I**, as two of the proximate atoms are identical. In sphere **II**, however, the atoms attached to the two carbon atoms ‘C-1’ and ‘C-3’ are ‘O,H,H’ and ‘H,H,H’, respectively, and, since ‘O > H’, the order of precedence is ‘C-l > C-3’ and hence the group ‘–CH_2OH’ is ‘b’ and the group ‘–CH_3’ is ‘c’, leading to the preferred IUPAC name:

(2*R*)-2-chloropropan-1-ol (PIN)

Example 2:

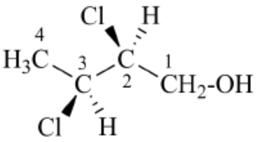


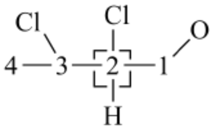

simplified digraph

Explanation: In the above compound, no decision is reached after the exploration of sphere **I**, since ‘Cl > C = C > H’. In sphere **II**, a decision is reached since ‘Cl > O’ and therefore the ‘–CH_2Cl’ group is ‘b’ and the group ‘–CH_2OH’ group is ‘c’, leading to the preferred IUPAC name:

(2*S*)-2,3-dichloropropan-1-ol (PIN)

Example 3:





simplified digraph for ‘2’

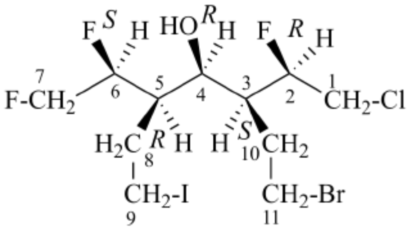
Explanation: In this example, two stereogenic centers are present in the molecule; therefore two digraphs are necessary, one for each stereogenic center. The digraph for the stereogenic atom at position 2 shows the ranking ‘Cl > C-3 > C-1 > H’ leading to a ‘*S*’ configuration for ‘C-2’. The digraph for the stereogenic atom at position 3 shows the ranking ‘Cl > C-2 > C-4 > H’ leading to a ‘*S*’ configuration for ‘C-3’ and the preferred IUPAC name:

(2*S*,3*S*)-2,3-dichlorobutan-1-ol (PIN)

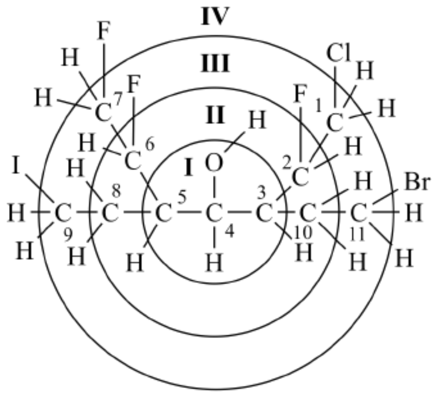
P-92.2.1.1.3 Beyond spheres **I** and **II**

When choices remain after evaluating the second sphere, the exploration procedure is continued in the same way further away from the stereogenic center.

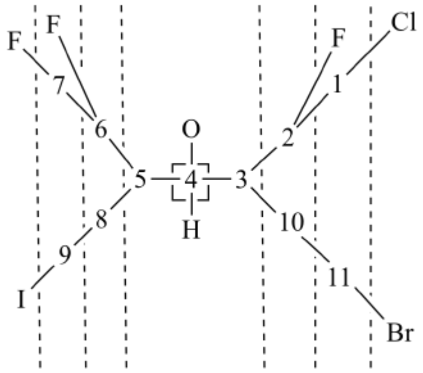
Example 1



(2*R*,3*S*,4*R*,5*R*,6*S*)-3-(2-bromoethyl)-1-chloro-2,6,7-trifluoro-5-(2-iodoethyl)heptan-4-ol (PIN)



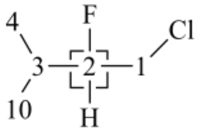
complete hierarchial digraph



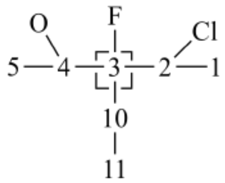
simplified digraph

Explanation: The first level of the exploration, sphere **I**, leads to ‘O > C-3 = C-5 > H’; no decision can be made between the two carbon atoms. In sphere **II**, still no decision can be made, because of the two identical sets of ‘C,C,H’ atoms attached to the carbon atoms of sphere **I**. In sphere **III**, the two branches on the left side are ranked ‘F,C,H’ > ‘C,H,H’; on the right side, the two branches are ranked ‘F,C,H’ > ‘C,H,H’ and still no decision can be made, but the two branches can be ranked giving precedence in further exploration to the two branches denoted by ‘F,C,H’ over ‘C,H,H’. In sphere **IV**, the two branches having received precedence in sphere **III** are examined and a decision is reached, because ‘Cl,H,H’ has precedence over ‘F,H,H’. Accordingly, the branch on the right hand side, ‘C-3’, is assigned the priority ‘b’ and the branch on the left hand side ‘C-5’, gets priority ‘c’. In the branches of lower precedence in sphere **III**, there are an iodine atom and a bromine atom. The fact that iodine has priority over bromine is not taken into consideration, because a decision has already been reached.

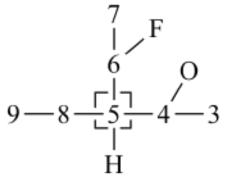
Hierarchial digraphs should be constructed for each stereogenic unit; however construction of a simple digraph and comparison of ligands can be parallel processes and frequently a partial digraph is enough to rank ligands. Partial digraphs for centers ‘C-2’ and ‘C-3’ to establish the configuration of these chirality centers are shown below. Similar digraphs must be constructed for ‘C-5’ and ‘C-6’.



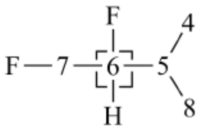
simplified digraph for ‘2’



simplified digraph for ‘3’

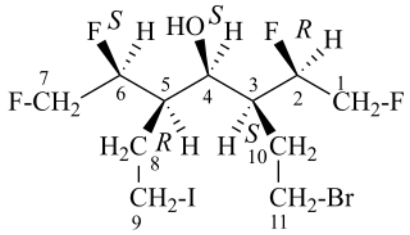


simplified digraph for ‘5’

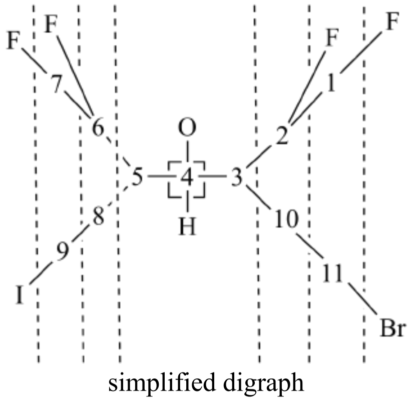


simplified digraph for ‘6’

Example 2



(2*R*,3*S*,4*S*,5*R*,6*S*)-3-(2-bromoethyl)-1,2,6,7-tetrafluoro-5-(2-iodoethyl)heptan-4-ol (PIN)



simplified digraph

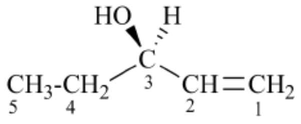
Note: This alcohol is similar to that in Example 1 above with a modification on the principal chain in which a chlorine atom has been replaced by a fluorine atom at position 1. This modification leads to an inversion of configuration of ‘C-4’ as discussed below.

Explanation: At ‘C-4’, ranking ‘O > C-3 = C-5 > H’ is first established. The two higher branches ‘C-3,C-2,C-1’ and ‘C-5,C-6,C-7’ cannot be differentiated. In the lower branches ‘C-3,C-10,C-11’ and ‘C-5,C-8,C-9’ a decision can be reached since ‘I > Br’, thus establishing the ranking order ‘O > C-5 > C-3 > H’ and thus the ’*S*’ configuration for ‘C-4’.

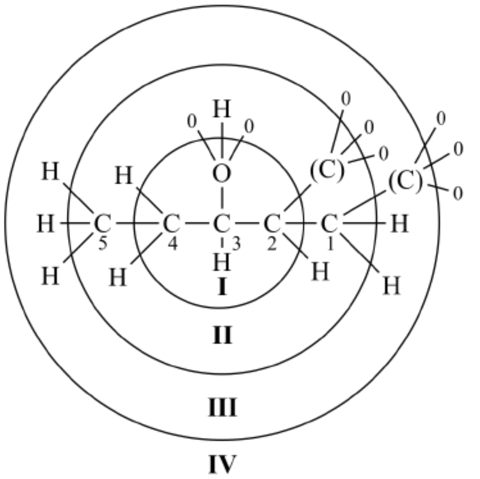
P-92.2.1.2 Double and triple bonds

Duplicate atom nodes as described in P-92.1.4.2 are used in digraphs.

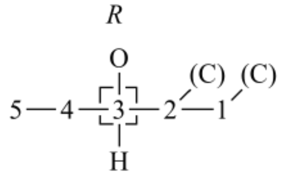
Example 1:



(3*R*)-pent-1-en-3-ol (PIN)



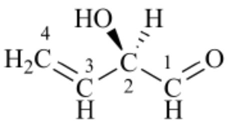
complete digraph



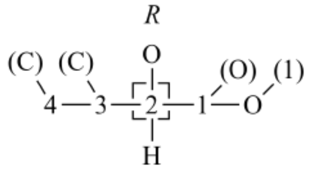
simplified digraph

Explanation: No decision can be reached in sphere **I**, in which ‘O > C-2 = C-4 > H’. In sphere **II**, (C) is a duplicate carbon atom, and ‘C,(C),H’ has priority over ‘C,H,H’ and the ranking of ligands is therefore ‘C-2 > C-4’, leading to an ‘*R*’ configuration for the chirality center ‘C-3’.

Example 2:



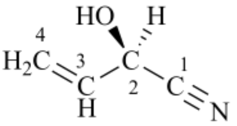
(2*R*)-2-hydroxybut-3-enal (PIN)



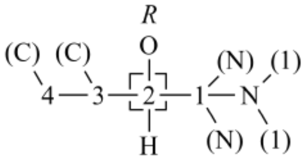
simplified digraph

Explanation: In sphere **I**, the priority is established as ‘O > C-1 = C-3 > H’ in accordance with Sequence Rule **1**. In sphere **II**, ‘C-1 > C-3’ because ‘O,(O),H’ for the –C=O group is senior to ‘C,(C),H’ for the –CH=CH$_2$ group, establishing the final ranking as ‘O > C-1 > C-3 > H’ and an ‘*R*’ configuration for the stereogenic center.

Example 3:



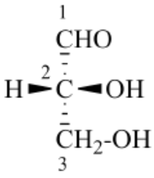
(2*R*)-2-hydroxybut-3-enenitrile (PIN)



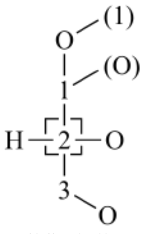
simplified digraph

Explanation: In sphere **I**, the priority is established as ‘O > C-1 = C-3 > H’ in accordance with Sequence Rule **1**. In sphere **II**, ‘C-1 > C-3’ because ‘N,(N),(N)’, for the –C≡N group, is senior to ‘C,(C),H’ for the $–CH=CH_2$ group, establishing the final ranking as ‘O > C-1 > C-3 > H’ and an ‘*R*’ configuration for the stereogenic center.

Example 4:



(2*R*)-2,3-dihydroxypropanal (PIN)



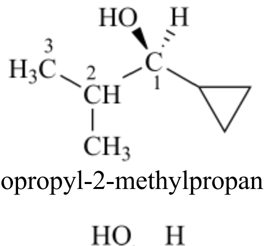
simplified digraph

Explanation: In sphere **I** priority order established is ‘O > C-1 = C-3 > H’ in accordance Sequence Rule **1**. In sphere **II**, ‘O,(O),H’ for the –CH=O group has priority over ‘O,H,H’ for the $–CH_2OH$ group; thus establishing the final ranking as ‘O > C-1 > C-3 > H’.

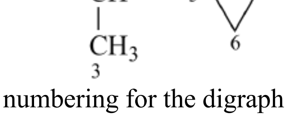
P-92.2.1.3 Saturated rings and ring systems

Duplicate atoms as described in P-92.1.4.3 are used in digraphs.

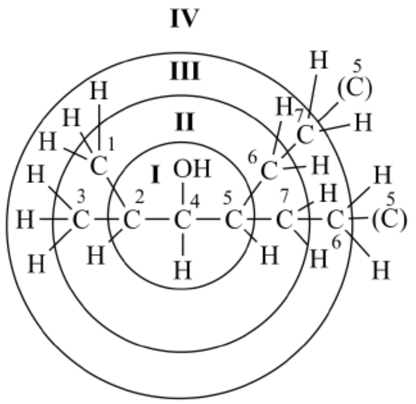
Example 1 (compare with example 3, below):



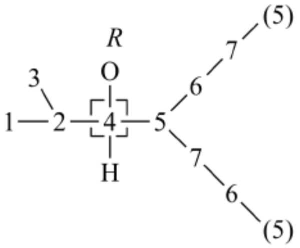
(1*R*)-1-cyclopropyl-2-methylpropan-1-ol (PIN)



numbering for the digraph



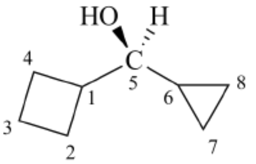
complete digraph



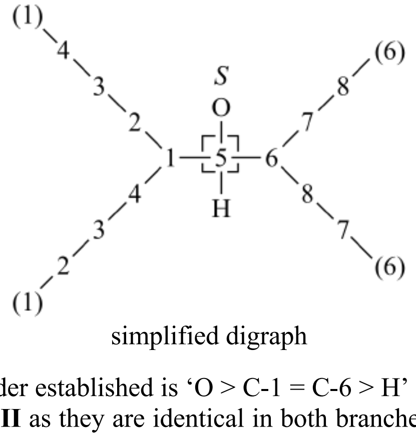
simplified digraph

Explanation: In sphere **I**, the priority order established is ‘O > C-5 = C-2 > H’ in accordance with Sequence Rule **1**. No decision is achieved in sphere **II** because the atoms bonded to both the ‘C-2 (C-1 and C-3)’ and ‘C-5 (C-6 and C-7)’ branches are ‘C,C,H’. However, in sphere **III**, both carbons bonded to ‘C-5 (C-6 and C-7)’ have ‘C,H,H’ ranking while both carbon atoms bonded to ‘C-2 (C-1 and C-3)’ have only a ‘H,H,H’ ranking; therefore the ‘C-5’ branch has priority over the ‘C-2’ branch resulting in the overall ranking of ‘O > C-5 > C-2 > H’ and an ‘*R*’ configuration for the stereogenic center.

Example 2



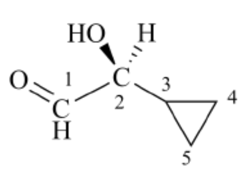
(*S*)-cyclobutyl(cyclopropyl)methanol (PIN)
(arbitrary numbering corresponding to the simple digraph)



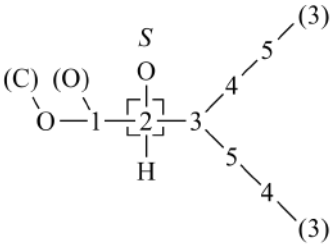
simplified digraph

Explanation: In sphere **I** the priority order established is ‘O > C-1 = C-6 > H’ in accordance with Sequence Rule **1**. No decisions can be made in spheres **II** or **III** as they are identical in both branches of the digraphs. In sphere **IV** there are only carbon atom nodes, and no decision can be reached. However, in the right branch there are only duplicated atoms and the left branch has nonduplicated atoms. Comparing atoms bonded to them in sphere **V**, there is nothing bonded to the duplicated atom and to the nonduplicated atom, ‘(C),H,H’. Since ‘(C),H,H’ has priority over “nothing”, the ‘C-1’ branch has priority over the C-6 branch, thus establishing the overall ranking ‘O > C-1 > C-6 > H’ and an ‘*S*’ configuration for the stereogenic center.

Example 3:

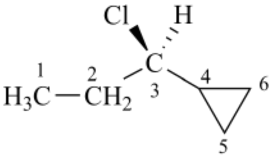


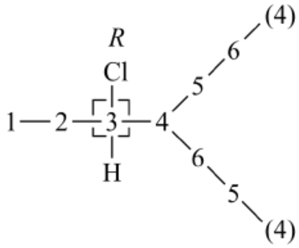
(*S*)-cyclopropyl(hydroxy)acetaldehyde (PIN)
(arbitrary numbering corresponding to the simple digraph)


simplified digraph

Explanation: In sphere **I** the priority order established is ‘O > C-1 = C-3 > H’ in accordance with Sequence Rule **1**. Here, in sphere **II**, the ranking in branch ‘C-1’ is ‘O,(O),H’ but in the C-3 branch it is ‘C,C,H’, leading to the overall ranking of ‘O > C-1 > C-3 > H’ and an ‘*S*’ configuration at the stereogenic center.

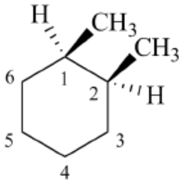
Example 4 (compare with example 1 above):

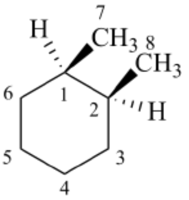

[(1*R*)-1-chloropropyl]cyclopropane (PIN)
(arbitrary numbering corresponding to the simple digraph)

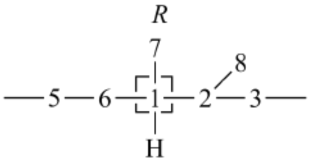

simplified digraph

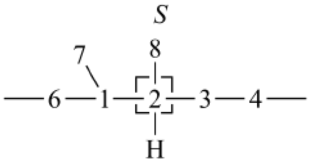
Explanation: In sphere **I** the priority order established is ‘Cl > C-4 = C-2 > H’ in accordance with Sequence Rule **1**. Here, in sphere **II**, the ranking in branch ‘C-4’ is ‘C,C,H’ but in the C-2 branch it is ‘C,H,H’, leading to the overall ranking of ‘Cl > C-4 > C-2 > H’ and an ‘*R*’ configuration at the stereogenic center.

Example 5:


(1*R*,2*S*)-1,2-dimethylcyclohexane (PIN)


(arbitrary numbering corresponding to the simple digraph)


simplified digraph for stereogenic atom C-1

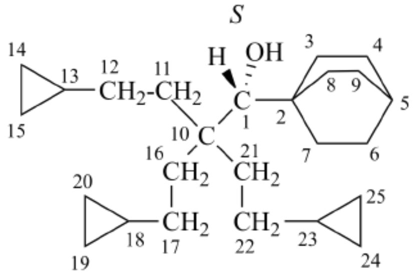

simplified digraph for stereogenic atom C-2

Explanation: In the procedure for specification of the configuration at ‘C-1’, in sphere **I** the priority order is ‘C-2 = C-6 = C-7 > H’ in accordance with Sequence Rule **1**. In sphere **II**, ‘C-2’ is bonded to two carbon atoms and one hydrogen atom, implicit in the digraph, ‘C,C,H’; C-6 is bonded to one carbon atom and to two hydrogen atoms, implicit in the digraph,‘C,H,H’, and there are three hydrogen atoms contributed by the C-7 group, ‘H,H,H’. Hence, the priority order for determining the configuration at C-1 is ‘C,C,H’ > ‘C,H,H’ > ‘H,H,H’ leading to the overall priority of ‘C-2 > C-6 > C-7 > H’ and the configuration ‘*R*’ at the stereogenic center ‘C-1’. For the specification of the configuration at ‘C-2’ the procedure is the same resulting in the priority order ‘C-1 > C-3 > C-8 > H’ and the configuration ‘*S*’ at the stereogenic center ‘C-2’.

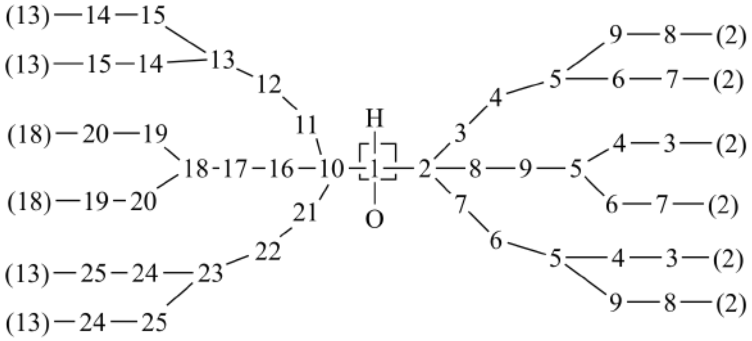
P-92.2.2 Sequence Subrule **1b**: Priority due to duplicate atoms

Custer (ref. 42) proposed an amendment to Sequence Subrule **1a** to establish the priority between substituents which give the same exploratory pathway according to rule **1a**. The subrule is based on the use of duplicate atoms and is expressed as ‘a duplicate atom corresponding to an atom closer to the start of the exploration pathway precedes one further away’ or more briefly ‘a nearer duplicate atom node takes precedence over a further away duplicate atom node’. The following examples illustrate this subrule.

Example 1:



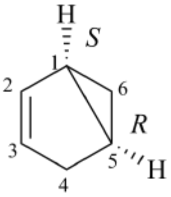
(1*S*)-1-(bicyclo[2.2.2]octan-1-yl)-4-cyclopropyl-2,2-bis(2-cyclopropylethyl)butan-1-ol (PIN)
(the numbering shown corresponds to the simplified digraph below)



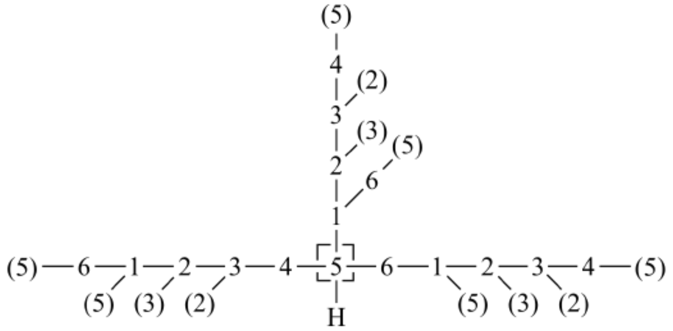
simplified digraph

Explanation: All four ligands from ‘C-1’ are different but those at ‘C- 2’ and ‘C-10’ are identical in the digraph. However, the duplicate atoms on the right correspond to the carbon in the first sphere (‘C-2’ of the bicyclo[2.2.2]octan-1-yl) whereas those on the left correspond to atoms at the fourth sphere (‘C-13’, ‘C-18’, and ‘C-23’ of the cyclopropyl groups). Since nearer duplicate atom nodes take precedence over atom nodes further away from the root of the digraph, ‘C-1’, the ranking is ‘O > C-2 > C-10 > H’ and a configuration ‘*S*’ for the stereogenic center ‘C-l’.

Example 2:



(1*S*,5*R*)-bicyclo[3.1.0]hex-2-ene (PIN)



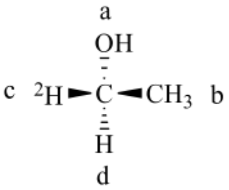
R
simplified digraph

Explanation. When comparing the 'C-4' and 'C-6' ligands, they are similar, except that the first duplicate atom on the right (bonded to C-1) corresponds to the stereogenic center, whereas the first one on the left (bonded to 'C-3') corresponds to atoms at the third sphere '(C-2)'. Since a duplicate atom corresponding to an atom closer to the start of the exploration pathway precedes one that is further away, the final ranking is 'C-1 > C-6 > C-4 > H' and the configuration '*R*' for the stereogenic center 'C-5'. The digraph permits the highest priority to be given to ligand 'C-1' and the lowest to 'H'.

P-92.3 SEQUENCE RULE **2**. Higher atomic mass number precedes lower atomic mass number.

When isotopes are present in a molecule, Sequence Rule **1** is first applied ignoring isotopic differences between otherwise identical atoms or groups. When no decision can be reached isotopes are then taken into consideration, arranged in decreasing order of their atomic mass, i.e. '$^{3}H > {}^{2}H > {}^{1}H$ (or H)' and '$^{81}Br > Br > {}^{79}Br$'.

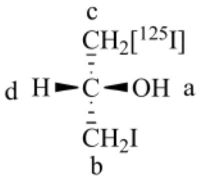
Example 1:



(1*R*)-(1-$^{2}H_{1}$)ethan-1-ol (PIN)

Explanation: The ranking order, 'a > b > c > d', after application of Sequence Rule **2**, is: '$O > C > {}^{2}H > H$' and the configuration is '*R*' for the stereogenic center.

Example 2:



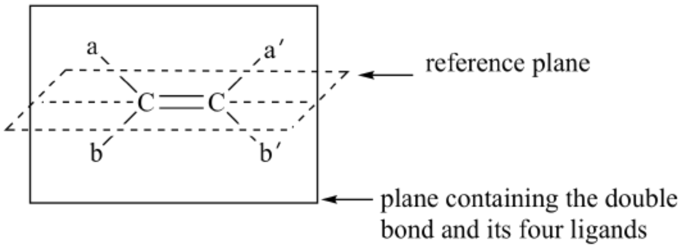
(2*S*)-1-[^{125}I]iodo-3-iodopropan-2-ol (PIN)

Explanation: The ranking order 'a > b > c > d', after application of Sequence Rule **2**, is: '$OH > CH_2I > CH_2[^{125}I] > H$' and the configuration is '*S*' for the stereogenic center.

P-92.4 SEQUENCE RULE **3**

P-92.4.1 '*seqcis*' = '*Z*' and '*seqtrans*' = '*E*'

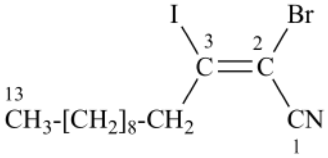
The descriptors '*E*' and '*Z*' are used to describe '*cis/trans*-isomers' at diastereomorphic double bonds. The atom or group having CIP Sequence Rule precedence attached to one of a doubly bonded pair of atoms is compared with the atom or group having CIP Sequence Rule precedence attached to the other atom; if the atoms or groups having precedence are on the same side of the reference plane, the italic capital letter '*Z*' is used as a stereodescriptor; if the atoms or groups having precedence are on opposite sides, the italic capital letter '*E*' is used. These stereodescriptors have been coined from German; '*Z*' is derived from 'zusammen' (together) and '*E*' from 'entgegen' (opposite).


a
a′
b
b′
C=C
reference plane
plane containing the double bond and its four ligands

The ‘*E*’ and ‘*Z*’ stereodescriptors have been classified in P-91.2.1 as non-CIP stereodescriptors. The reason is that they do not distinguish between geometrically diasteromorphic double bonds whose descriptors are reflection invariant (‘common’ double bonds) from the geometrically enantiomorphic double bonds whose stereodescriptors are reflection variant. In the CIP system, reflection variant descriptors are capitalized (for example ‘*R*’ and ‘*S*’) and reflection invariant descriptors are lower-case descriptors (for example ‘*r*’ and ‘*s*’). The fact that ‘*E*’ and ‘*Z*’ are capitalized is contrary to their reflection invariant status. Hirschman and Hanson (ref. 43) proposed to use the descriptors ‘*seqcis*’, ‘*seqtrans*’, ‘*seqCis*’, and ‘*seqTrans*’ as CIP descriptors.

When discussing configuration assignment, the CIP descriptors are used, with the understanding that ‘*seqcis*’ = ‘*Z*’, and ‘*seqtrans*’ = ‘*E*’. In names, the descriptors ‘*E*’ and ‘*Z*’ are used, with the additional difficulty that the traditional ‘*cis*’ relationship is ‘senior to ‘*trans*’ relationship in the numbering of compounds containing diasteromorphic double bonds is translated into ‘*Z*’ is senior to ‘*E*’, irrespective of the alphabetical order.

Example:


I
Br
3
2
C=C
13
CH3-[CH2]8-CH2
CN
1

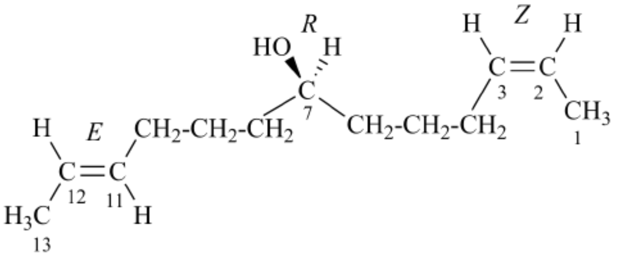
(2*Z*)-2-bromo-3-iodotridec-2-enenitrile (PIN)

Explanation: In this compound, application of Sequence Rule **1** described in P-91.2.1 gives precedence to ‘I’ over the carbon chain in position ‘3’; similarly, in position 2, ‘Br’ has precedence over the ‘C’ of the CN group. Thus the configuration of the double bond is ‘*Z*’, the atoms ‘I’ in position ‘3’ and ‘Br’ in position ‘2’ being compared.

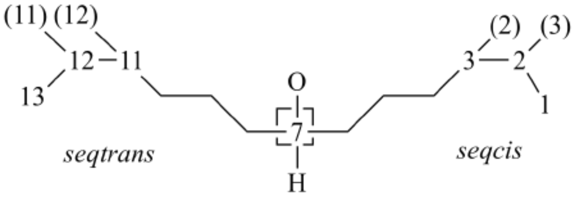
P-92.4.2 Sequence Rule **3**: ‘*seqcis*’ (‘*Z*’) precedes ‘*seqtrans*’ (‘*E*’) and this order precedes nonstereogenic double bonds

P-92.4.2.1 The application of Sequence Rule **3** leads to the specification of the configuration of compounds containing sets of ‘*cis*’ and ‘*trans*’ double bonds when the direct application of Sequence Rules **1** or **2** does not permit a conclusion to be reached (see Mata, Lobo, Marshall, and Johnson, ref. 41).

Example 1:

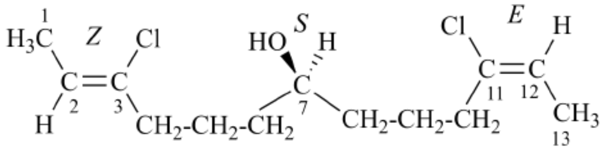

R
HO
H
C
7
H
Z
H
C=C
3
2
CH3
1
H
E
CH2-CH2-CH2
CH2-CH2-CH2
C=C
12
11
H3C
H
13

(2*Z*,7*R*,11*E*)-trideca-2,11-dien-7-ol (PIN)

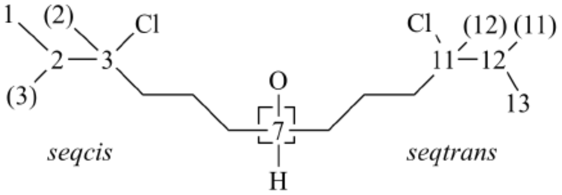

(11) (12)
12—11
13
O
7
H
(2) (3)
3—2
1
seqtrans
seqcis

simplified digraph for establishing the ranking *seqcis* = (*Z*) > *seqtrans* = (*E*)
and the ‘*R*’ configuration for ‘C-7’

Example 2:


1
H3C
Z
Cl
C=C
2
3
H
CH2-CH2-CH2
S
HO
H
C
7
Cl
E
H
C=C
11
12
CH2-CH2-CH2
CH3
13

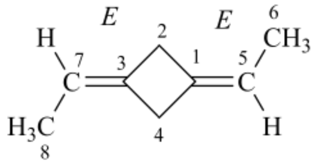
(2*Z*,7*S*,11*E*)-3,11-dichlorotrideca-2,11-dien-7-ol (PIN)



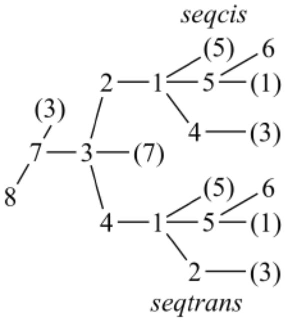
simplifed digraph for establishing the ranking *seqcis* (*Z*) > *seqtrans* (*E*)
and the '*S*' configuration for 'C-7'

P-92.4.2.2 Auxiliary stereodescriptors are used when direct assignment of configuration cannot be made to double bonds. In the following example, the four-membered ring is opened to generate a digraph as discussed in P-92.2.1.3, thus creating two branches each containing a double bond whose configuration is '*seqcis*' (*Z*) in one case and '*seqtrans*' (*E*) in the other considering the ligands as they appear in the digraph. The assignment of these stereodescriptors is transitory, but permits a definitive configuration to be assigned to the remaining double bond located at 'C-3' by using the Sequence Rule **3**, '*seqcis* > *seqtrans*'. The definitive stereodescriptor is thus '*E*' for the ethylidene substituent located at position '1', and also '*E*' for the ethylidene group located at position '3'.

Example 1:



(1*E*,3*E*)-1,3-diethylidenecyclobutane (PIN)
1,3-di[(*E*)-ethylidene]cyclobutane
(*E*)-1,3-diethylidenecyclobutane

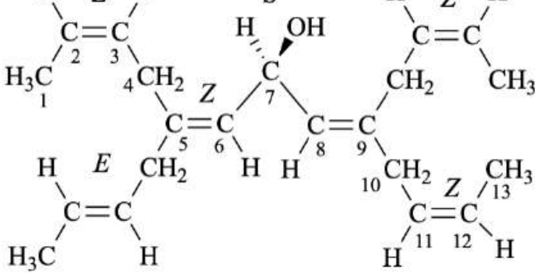


simplified digraph

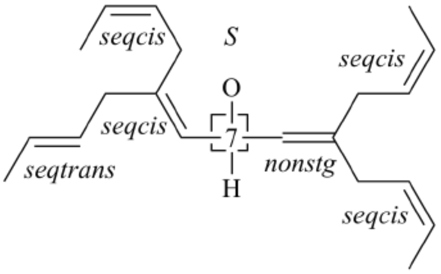
Explanation: To specify double bonds, ligands of both double bond atoms should be ranked. This is straightforward for the ligands of 'C- 5' and 'C-7'. However the ranking of ligands at 'C-1' and 'C-3' is a complex process, and requires the use of auxiliary descriptors. The following digraph, with a specific numbering, shows configuration '*E*' at 'C-3'. As the digraph is acyclic, it is possible to specify the double bond 'C-1', using the ligands as they appear in the digraph. These are auxiliary descriptors that are different in branches 'C-2' and 'C-4' and allow the ligands to be ranked, 'C-2 > C-4'.

In names, the stereodescriptor '*E*' is used to describe each double bond; the two stereodescriptors are placed at the front of the name, in parentheses, each preceded by the locant indicating the position of the double bond on the ring. This method is used in preferred IUPAC names. It is preferred to the method which attributes the double bond to the substituent group and cites the required stereodescriptor(s) at the front of the substituent group. A third method considers that the stereodescriptor '*E*' describes the whole molecule, considered as an extended double bond.

Example 2:



(2*Z*,5*Z*,7*S*,11*Z*)-5-[(2*E*)-but-2-en-1-yl]-9-[(2*Z*)-but-2-en-1-yl]trideca-2,5,8,11-tetraen-7-ol (PIN)



simplified digraph showing stereogenic (*seqcis* and *seqtrans*) and nonstereogenic (*nonstg*) units

Explanation: When comparing double bonds the first to be compared (starting from the core of the digraph) are the ‘C-5’ double bond that is ‘*seqcis*’ and the ‘C-9’ double bond that is nonstereogenic. As a ‘*seqcis*’ configuration precedes a nonstereogenic one, the ranking of the ligands is: ‘OH > C-6 > C-8 > H’ and the configuration of the chirality center is ‘*S*’.

P-92.5 SEQUENCE RULE **4**

When the use of Sequence Rules **1**, **2**, and **3** does not permit the determination of the ranking of all ligands of a stereogenic unit, Sequence Rule **4** is applied as described here. For the purpose of this Section, Sequence Rule **4** is simplified and discusses only the stereodescriptors most encountered in nomenclature of organic compounds, i.e. ‘*R*’, ‘*S*’, ‘*r*’, and ‘*s*’.

It is important to note that full digraphs are necessary for the analysis of all stereogenic units. Descriptors specified in digraphs may correspond to the final descriptors or to temporary (auxiliary) descriptors used only for ranking ligands and never appearing as final descriptors.

A simplified version of Sequence Rule **4** that only considers stereogenic centers is expressed as follows:

(a) chiral stereogenic units precede pseudoasymmetric stereogenic units and these precede nonstereogenic units;

(b) When two ligands have different descriptor pairs, then the one with the first chosen *like* descriptor pairs has priority over the one with a corresponding *unlike* descriptor pair:

(i) *Like* descriptor pairs are: ‘*RR*’, ‘*SS*’;

(ii) *Unlike* descriptor pairs are ‘*RS*’, ‘*SR*’;

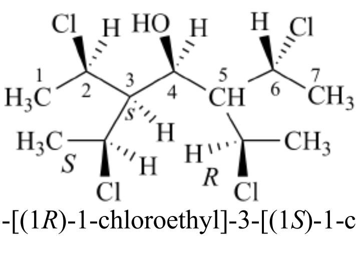
(c) ‘*r*’ precedes ‘*s*’.

It is convenient to divide Sequence Rule **4** into three subrules.

P-92.5.1 Sequence Rule **4a**

Chiral stereogenic units precede pseudoasymmetric stereogenic units and these precede nonstereogenic units.

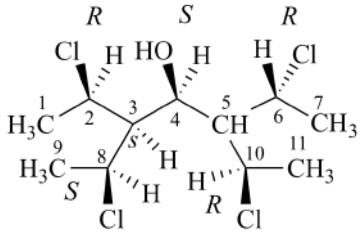
Example:



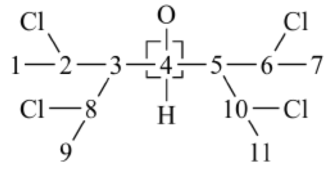
(2*R*,3*s*,4*S*,6*R*)-2,6-dichloro-5-[(1*R*)-1-chloroethyl]-3-[(1*S*)-1-chloroethyl]heptan-4-ol (PIN)

Note: The numbering of the principal chain is based on lowest locants for stereogenic centers; the stereodescriptor set ‘2*R*,4*S*,6*R*’ in the principal chain is preferred to ‘2*S*,4*S*,6*R*’ according to Sequence Rule **5** (see P-92.6).

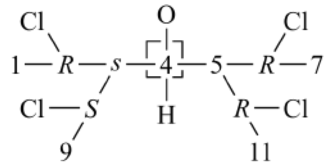
Explanation: The molecule is renumbered in preparation for the construction of digraphs. According to P-92.1.4.1 digraphs of all stereogenic centers are constructed, thus allowing the specification at ‘C-2’, ‘C-6’, ‘C-8’, and ‘C-10’. Digraphs are also constructed for specifying the configuration of ‘C-3’ and ‘C- 5’. The configuration at ‘C-2’, ‘C-6’, and ‘C-10’ is determined as ‘*R*’ by applying Sequence Rule **1**; the configuration at ‘C-8’ is ‘*S*’ by applying the same rule. The configuration at ‘C-3’ is determined as ‘*s*’ by ranking two of the ligands by Sequence Rule **5** (see below, ‘*R*’ precedes ‘*S*’); ‘C-5’ is a nonstereogenic center as it is substituted by two identical groups (both chirality centers are ‘*R*’). The simple digraphs needed for the specification of ‘C-4’ are shown below.



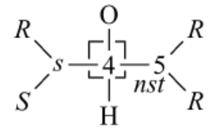
arbitrary renumbered molecule for the simplified digraphs below.



simplified digraph



a first simplified digraph modified by introducing configurations at ‘C-2’, ‘C-3’, ‘C-6’, ‘C-8’, and ‘C-10’, as determined above.



further simplified digraph to show the relevant information necessary to determine the configuration at ‘C-4’.

Explanation: Final simplified digraph showing that the four ligands around the stereogenic unit ‘C-4’ are different and can be ranked: ‘OH > pseudoasymmetric stereogenic unit > nonstereogenic unit (nst) > H’. Hence, the configuration for ‘C-4’ is ‘*S*’.

P-92.5.2 Sequence Rule **4b**

When two ligands have different descriptor pairs, then the one with the first chosen *like* descriptor pairs has priority over the one with a corresponding *unlike* descriptor pair.

(i) *Like* descriptor pairs are: ‘*RR*’, ‘*SS*’:

(ii) *Unlike* descriptor pairs are: ‘*RS*’, ‘*SR*’

P-92.5.2.1 Methodology for pairing ligands

A new methodology has recently been described by Mata and Lobo (ref. 41) to replace that described by Prelog and Helmchen (see subsection 5.4, ref. 36). The rule for pairing stereodescriptors is as follows: A reference descriptor for chirality centers, identified as ***R*** or ***S*** (not associated with any node of the digraph and designated here with a bold font), is chosen in each ligand and is:

(a) the one associated with the highest rank node corresponding to a chiral unit in the ligand;

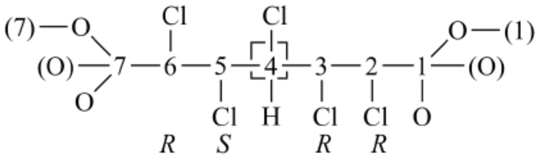
(b) the one that occurs the most in the set of equivalent highest rank nodes; or

(c) sequentially both descriptors (***R*** and ***S***), if these occur in the same number in the set of equivalent highest ranked nodes:

(i) If the number of reference descriptors is different in both ligands then the ligand with one reference descriptor has priority over the one with two reference descriptors;

(ii) If both ligands have the same number of reference descriptors, then the reference descriptor is paired with each one of the descriptors, identified as *R* or *S*, associated with nodes corresponding to chiral units, respecting their connectivity and hierarchy in the digraph.

In the following digraph (see example 1 in P-92.5.2.2) the configuration at ‘C-4’ is determined by the four ligands ‘Cl’, ‘H’ and the two branches ‘C-3,C-2,C-1’ (right branch) and ‘C-5,C-6,C-7’ (left branch)’ showing the connectivity and the hierarchical order of nodes.

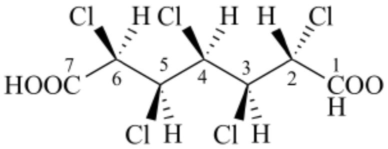


simplified digraph

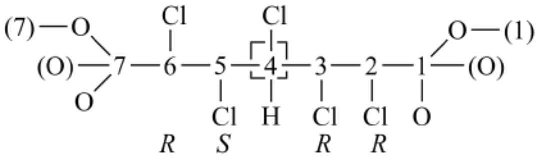
The descriptors ‘*R*’ and ‘*S*’ shown in the digraph for chirality centers at ‘C-2’, ‘C-3’, ‘C-5’, and ‘C-6’ are determined by Sequence Rule **1**; the reference descriptors ‘***R***’ or ‘***S***’ are chosen according to the hierarchical order of nodes, ‘C-3’ for the right branch and ‘C-5’ for the left branch; thus ‘***R***’ is chosen for the right branch, as ‘C-3’ is ‘*R*’; the descriptor ‘***S***’ is chosen for the left branch, as ‘C-5’ is ‘*S*’. Then, the pair ‘***R****R*’ is established for the nodes ‘C-3’ and ‘C-2’; the pair ‘***S****S*’ is established for node ‘C-5’ and the pair ‘***S****R*’ for the node ‘C-6’. The pairs ‘***R****R*’and ‘***S****S*’ are *like* descriptor-pairs; the pairs ‘***S****R*’ and ‘***R****S*’ are *unlike* descriptors-pairs. The Sequence Rule **4** is applied to pairs containing the reference descriptors; they are compared in the hierarchical order of their nodes, ‘C-3’ and ‘C-5’, then ‘C-2’ and ‘C- 6’. No decision can be reached by the comparison of the two *like* pairs ‘***R****R*’ at ‘C-3’ and ‘***S****S*’ at ‘C-5’; the comparison between the *like* pair ‘***R****R*’ at ‘C-2’ and the *unlike* pair ‘***S****R*’ at ‘C-6’ leads to the decision the branch with the *like* pair has priority over the branch with the *unlike* pair. The final order of ligands ‘Cl > C-3 > C-5 > H’ determines the ‘*R*’ configuration for the chiral center ‘C-4’.

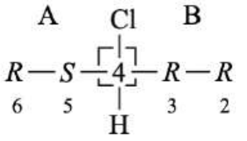
P-92.5.2.2 Application of the methodology in P-92.5.2.1 is illustrated by the following examples; the criteria in P-92.5.2.1 are applied in the order (a), (b), (c), (i), and (ii) as required. Examples 1 through 4 are related to criterion (a); example 5 to criterion (b); example 6 to subcriterion (i) following (c). Example 6 in P-92.6 illustrates criterion (c).

Example 1:



(2*R*,3*R*,4*R*,5*S*,6*R*)-2,3,4,5,6-pentachloroheptanedioic acid (PIN)





reference descriptor

S ***R***

pairs of descriptors

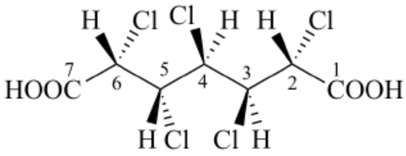
$S,5 \longrightarrow l \qquad R,3 \longrightarrow l$

$S,6 \longrightarrow u \longleftrightarrow R,2 \longrightarrow l$

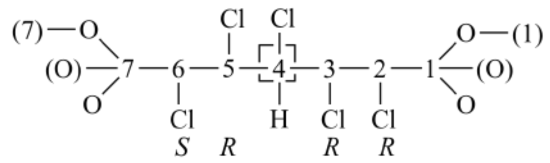
A < B

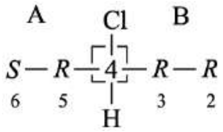
Explanation: In this example, the configuration at ‘C-2’, ‘C-3’, ‘C-5’, and ‘C-6’ is determined by the ranking of the ligands by Sequence Rule **1**. In each branch (ligand) A and B of the digraph, the highest ranked node is chosen as reference descriptor, ‘***R***’ for the B branch and ‘***S***’ for the A branch. Pairs of descriptors are formed by pairing the reference descriptor and each descriptor (denoted by its locant) starting from the core of the digraph; they are described as ‘*l*’ or ‘*u*’, *like* pairs being ‘***R****R*’ or ‘***S****S*’, *unlike* pairs being ‘***R****S*’ or ‘***S****R*’. The comparison of pairs between branches is achieved according to the decreasing hierarchical ranking. At the first difference, the *like* pair has precedence over the *unlike* pair, leading to the ‘*R*’ configuration for ‘C-4’.

Example 2:



(2*R*,3*R*,4*R*,5*R*,6*S*)-2,3,4,5,6-pentachloroheptanedioic acid (PIN)





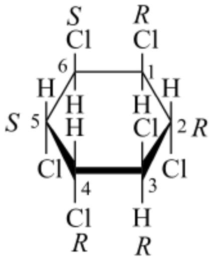
reference descriptor
R ***R***

pairs of descriptors
R,5 → *l* *R*,3 → *l*
R,6 → *u* ↔ *R*,2 → *l*

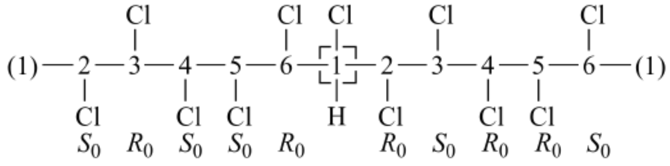
A < B

Explanation: In this example, the configuration at ‘C-2’, ‘C-3’, ‘C'-5’, and ‘C-6’ is determined by application of Sequence Rule **1**. In each branch (ligand) A and B of the digraph, the highest ranked node is chosen as reference descriptor, ‘***R***’ for the two branches. Pairs of descriptors are formed by pairing the reference descriptor and each descriptor (denoted by its locant) starting from the core of the digraph; they are described as ‘*l*’ or ‘*u*’, *like* pairs being ‘***RR***’ or ‘***SS***’, *unlike* pairs being ‘***RS***’ or ‘***SR***’. The comparison of pairs between branches is achieved according to the decreasing hierarchical ranking. At the first difference, the *like* pair has precedence over the *unlike* pair, leading to the ‘*R*’ configuration for ‘C-4’.

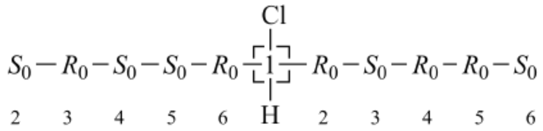
Example 3.



(1*R*,2*R*,3*R*,4*R*,5*S*,6*S*)-1,2,3,4,5,6-hexachlorocyclohexane (PIN)



digraph for the determination of the configuration at C-1
based on the numbering shown above



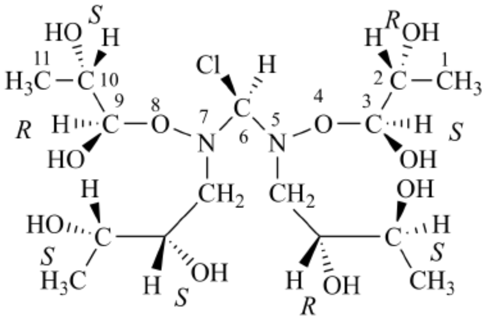
reference descriptor
R ***R***

pairs of descriptors
R, 6 → *l* *R*, 2 → *l*
R, 5 → *u* *R*, 3 → *u*
R, 4 → *u* ↔ *R*, 4 → *l*
R, 3 → *l* *R*, 5 → *l*
R, 2 → *u* *R*, 6 → *u*

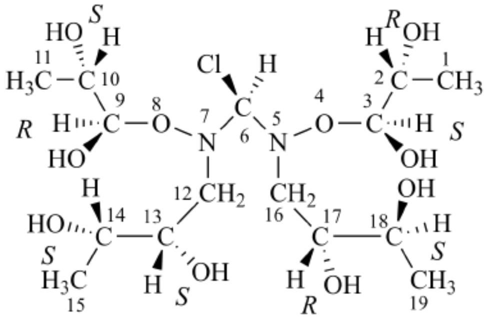
A < B

Explanation: This example illustrates the use of reference descriptors and that of auxiliary descriptors, R_0 and S_0, specified in place of usual stereodescriptors *R* and *S* as described by Prelog and Helmchen (see 6.2.1 in ref. 36). The first step consists in establishing a digraph showing auxiliary descriptors (R_0 and S_0) illustrated here for C-1. The auxiliary descriptors for every node are determined for this digraph. For example, the auxiliary descriptor for C-6 node is R_0 as Cl > C-1 > C5 > H. Once all necessary auxiliary descriptors are assigned, the methodology described by Mata and Lobo for pairing descriptors is then applied. In this example, reference descriptors are chosen in accordance with the highest ranked nodes in the A and B branches: both reference stereodescriptors are ‘*R*’. The analysis of the pairing of descriptors leads to the precedence of branch B over branch A, and the ‘*R*’ configuration for ‘C-1’.

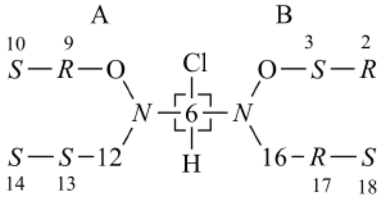
Example 4:


S
HO H
11
H3C—C 10
9
R H—C—O
HO
8
Cl H
7
C
N
6
5
4
N
R
H OH
1
2 C—CH3
3
O—C—H S
OH
CH2
CH2
H
HO
C
S
H3C
H
OH
S
OH
C—H
S
CH3
H OH
R

(2*R*,3*S*,6*R*,9*R*,10*S*)-6-chloro-5-[(2*R*,3*S*)-2,3-dihydroxybutyl]-7-[(1*S*,2*S*)-2,3-dihydroxybutyl]-4,8-dioxa-5,7-diazaundecane-2,3,9,10-tetrol (PIN;
in the principal chain, named by skeletal replacement nomenclature, both pairs of stereodescriptors are *unlike*;
so the stereodescriptor *R* is assigned to the lowest locant, ‘2’)


S
HO H
11
H3C—C 10
9
R H—C—O
HO
8
Cl H
7
C
N
6
5
4
N
R
H OH
1
2 C—CH3
3
O—C—H S
OH
12 CH2
CH2
H
14
13
HO
C—C
S
H3C
15
H
OH
S
16
17
C
H OH
R
OH
18
C—H
S
CH3
19

arbitrary numbering used in the construction of the digraph for at C-6


A
B
10 9
S—R—O
Cl
3 2
O—S—R
N—6—N
S—S—12
14 13
H
16—R—S
17 18

reference descriptor

R ***S***

pairs of descriptors

R, 9 $\longrightarrow l$ *S*, 3 $\longrightarrow l$

R, 13 $\longrightarrow u$ *S*, 17 $\longrightarrow u$

R, 10 $\longrightarrow u$ *S*, 2 $\longrightarrow u$

R, 14 $\longrightarrow u \longleftrightarrow$ *S*, 18 $\longrightarrow l$

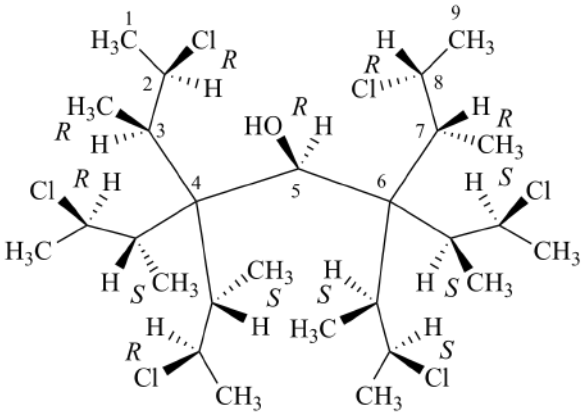
A < B

The seniority of B over A leads to the ‘*R*’ configuration for C-6.

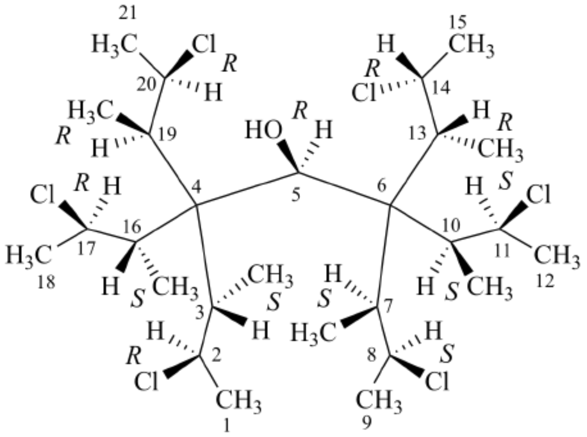
Explanation: First, the structure is renumbered as shown above. Then, the configurations at ‘C-2’, ‘C-3’, ‘C-9’, ‘C-10’, ‘C-13’, ‘C-14’, ‘C-17’, and ‘C-18’ are determined by the ranking of the ligands by Sequence Rule **1**. However, Sequence Rule **1** does not allow to rank two of the ligands of chirality center ‘C-6’, and pairs of descriptors of their chiral units are compared according to Sequence Rule **4**. The ranking of the chirality centers in both ligands of ‘C-6’, previously defined by the application of Sequence Rule **1**, is for branch A ‘C-9’ > ‘C-13’ > ‘C-10’, > ‘C-14’ and for branch B ‘C-3’ > ‘C-17’ > ‘C-2’, > ‘C-18’. The next step is to choose the reference descriptor ‘***R***’ or ‘***S***’, based on the one associated with the highest ranking chiral unit in each of the ligands. It is ‘***R***’ for branch A and ‘***S***’ for branch B. Finally the pairing of descriptors is made, respecting the connectivity and hierarchy in the digraph. At the first difference, the *like* pair has precedence over the *unlike* pair, thus establishing the precedence of branch B over branch A, leading to the configuration ‘*R*’ for ‘C-6.

Example 5:

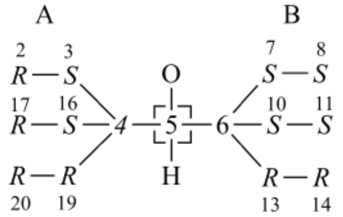
This example illustrates the application of criterion (b) of the rule described in P-92.5.2.1.



(2*R*,3*R*,5*R*,7*R*,8*R*)-2,8-dichloro-4,4-bis[(2*S*,3*R*)-3-chlorobutan-2-yl]-6,6-bis[(2*S*,3*S*)-3-chlorobutan-2-yl]-3,7-dimethylnonan-5-ol (PIN;
the principal chain contains two pairs of stereodescriptors, one *like*, the other *unlike*;
lowest locants are assigned to the *like* pair)



arbitrary numbering used in the construction of the digraph at ‘C-5’



reference descriptor

S **S**

pairs of descriptors

$$\begin{array}{lcl}
\left\{\begin{array}{l} S, 3 \rightarrow l \\ S, 16 \rightarrow l \end{array}\right. & & \left.\begin{array}{l} S, 7 \rightarrow l \\ S, 10 \rightarrow l \end{array}\right\} \\
\quad S, 19 \rightarrow u & & S, 13 \rightarrow u \\
\left\{\begin{array}{l} S, 2 \rightarrow u \\ S, 17 \rightarrow u \end{array}\right. & \longleftrightarrow & \left.\begin{array}{l} S, 8 \rightarrow l \\ S, 11 \rightarrow l \end{array}\right\} \\
\quad S, 20 \rightarrow u & & S, 14 \rightarrow u
\end{array}$$

final result

S *lluuuu* **S** *llullu*

A < B

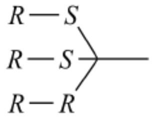
The seniority of B over A leads to the ‘*R*’ configuration for C-6.

Explanation: First the structure is renumbered as shown above. Then, configurations at ‘C-2’, ‘C-3’, ‘C-7’, ‘C-8’, ‘C-10’, ‘C-11’, ‘C-13’, ‘C-14’, ‘C-16’, ‘C-17’, ‘C-19’ and ‘C-20’ are established by the application of Sequence Rule **1**. Achiral centers are present at ‘C-4’ and ‘C-6’. The determination of the configuration at ‘C-5’ is illustrated below in accordance with the shown digraph. Next, the reference descriptors are chosen. In the left branch nodes in sphere **II** are hierarchically equivalent, two of them are ‘*S*’ and the other is ‘*R*’. Thus, the reference descriptor is ‘***S***’; it is the one that occurs most in the set of equivalent highest ranked nodes. Similarly, in the right branch the reference descriptor is ‘***S***’.

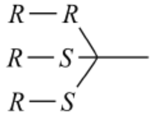
The hierarchy used in the comparison of the pairs of descriptors is established as follows. After reordering the three nodes in sphere **II** of the digraph (nodes bonded to 'C-4' in the left branch and to 'C-6' in the right branch), the nodes are no more equivalent. Those that form *like* pairs have precedence over the one that forms an *unlike* pair. Similarly, the ranking in branch B gives precedence to *like* pairs.

The analysis of the digraph leads to the conclusion that the comparison of pairs establishes, at the first difference, the priority of the pair *S*,8 and *S*,11 (*like pair*) over the pair *S*,2 and *S*,17 (*unlike pair*) leading to the priority of the branch B over the branch A, and to the configuration '*R*' at 'C-5'. The reordering of the digraph is always required when applying the Sequence Rules. Before comparison according to Sequence Rule **4b**, partial digraphs 1, 2, and 3 below (nodes at top of the digraph are equivalent or higher ranked than those nodes closer to the bottom of the digraph) are all valid to represent branch A. However, after comparison of sphere **II** only digraph 1 represents the hierarchy of the nodes.

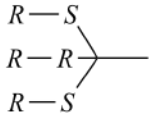
1



2

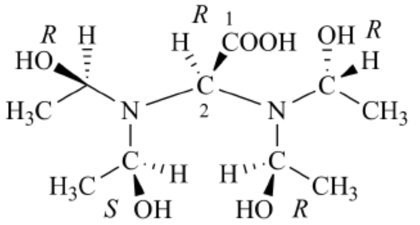


3

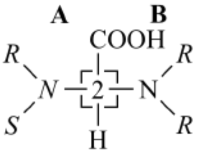


Example 6:

This example illustrates criterion (i) described in the methodology recommended by Mata and Lobo (see P-92.5.2.1), which is: If the number of reference descriptors is different in both ligands then the ligand with one reference descriptor has priority over the one with two reference descriptors.



(*R*)-{bis[(1*R*)-1-hydroxyethyl]amino}{[(1*R*)-1-hydroxyethyl][(1*S*)-1-hydroxyethyl]amino}acetic acid (PIN)

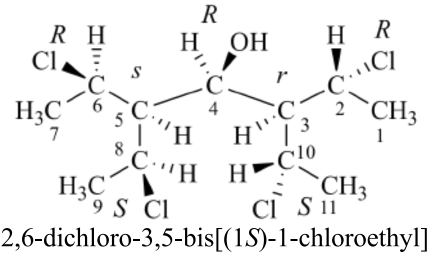


simplified digraph for the specification of the configuration at C-2

Explanation: In branch A, both descriptors ('***R***' and '***S***') are used as reference descriptors; in branch B, there is only one reference descriptors ('***R***'); thus, the ligand B ranks higher, leading to '*R*' configuration for 'C-2'.

P-92.5.3 Sequence Rule **4c**: '*r*' precedes '*s*'

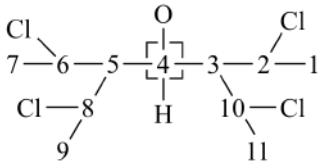
Example:



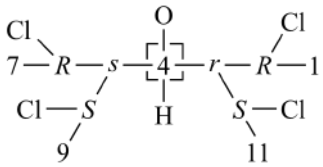
(2*R*,3*r*,4*R*,5*s*,6*R*)-2,6-dichloro-3,5-bis[(1*S*)-1-chloroethyl]heptan-4-ol (PIN)

Note: According to Sequence Rule **4a(b)** in P-92.5.2.1, the locant set '(2*R*,4*R*,6*R*)' has priority over '(2*R*,4*R*,6*S*)'. In the principal chain, the lower locant '3' is given to the pseudoasymmetric center '*r*').

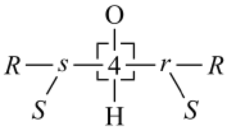
Explanation: The configuration at ‘C-2’ and ‘C-6’ is determined as ‘*R*’ by applying Sequence Rule **1**; by the same rule, the configuration is at ‘C-8’ and ‘C-10’ is ‘*S*’. The configuration at ‘C-5’ is determined as ‘*s*’ by applying Sequence Rule **5** (see below, ‘*R*’ precedes ‘*S*’); by the same rule the configuration at ‘C-3’ is ‘*r*’. By the procedure described in P-92.5.2.1 above, the following simplified digraphs are constructed:



a first simplified digraph is constructed



simplified digraph indicating the configuration
of the chiral and pseudoasymmetric centers

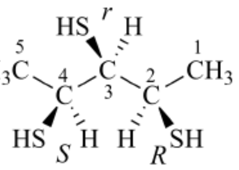


By applying the rule ‘*r*’ precedes ‘*s*’, the configuration at ‘C-4’ is ‘*R*’.

P-92.6 SEQUENCE RULE **5**: ‘*R*’ precedes ‘*S*’, ‘*M*’ precedes ‘*P*’, and ‘*seqCis*’ precedes ‘*seqTrans*’, and similarly for auxiliary descriptors.

In preferred IUPAC names the lower case stereodescriptors ‘*r*’ and ‘*s*’ are used to describe pseudoasymmetric centers, and ‘*m*’ and ‘*p*’ describe axial or planar pseudoasymmetry. These stereodescriptors are invariant on reflection. In contrast, two chiral ligands of opposite configuration on the same position of a double bond generate geometrically enantiomorphic double bonds denoted by the stereodescriptors ‘*seqCis*’ or ‘*seqTrans*’; such configurations are reflection-variant (see Example 5, below). For ‘*seqCis*’ precedes ‘*seqTrans*’ see Example 4 in P-93.5.1.4.2.2.

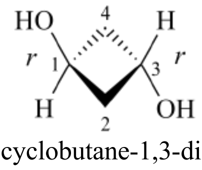
Example 1:



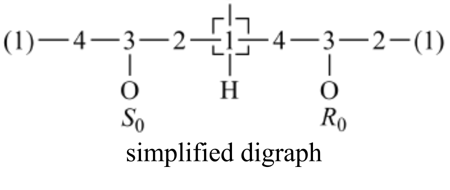
(2*R*,3*r*,4*S*)-pentane-2,3,4-trithiol (PIN)

Explanation: The configurations at ‘C-2’ and ‘C-4’ are determined by applying Sequence Rule **1**. The configuration ‘*r*’ at ‘C-3’ is arrived at in accordance with the sequence ‘S > C-2 > C-4 > H’.

Example 2:



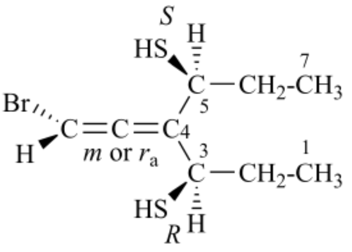
(1*r*,3*r*)-cyclobutane-1,3-diol (PIN)



simplified digraph

Explanation: The following digraph specifies the configuration ‘*r*’ for ‘C-1’, in accord with the rule ‘*R*’ precedes ‘*S*’. In the same way, configuration ‘*r*’ at C-3 is determined. Auxiliary descriptors ‘R_0’ and ‘S_0’ are used in place of usual descriptors specified by applying Sequence Rule **1** (see Prelog and Helmchen, subsection 6.2.1, ref. 36).

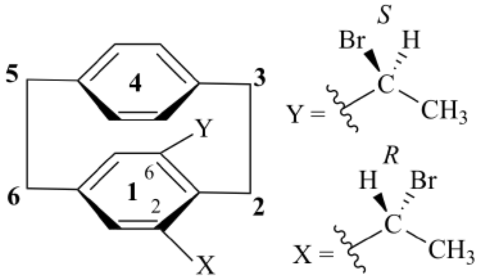
Example 3:


S
HS
H
7
C—CH$_2$-CH$_3$
5
Br
C=C=C4
H
m or r_a
3
1
C—CH$_2$-CH$_3$
HS
R
H

(3*R*,4*m*,5*S*)-4-(2-bromoethen-1-ylidene)heptane-3,5-dithiol (PIN)
(3*R*,4*r*$_a$,5*S*)-4-(2-bromoethen-1-ylidene)heptane-3,5-dithiol

Explanation: The configurations at 'C-3' and 'C-5' are determined by applying Sequence Rule **1**. The configuration '*m*' or '*r*$_a$' at 'C-4' is determined in accordance with the methodology described in P-92.1.2.1.2 (see also P-93.5.7.1).

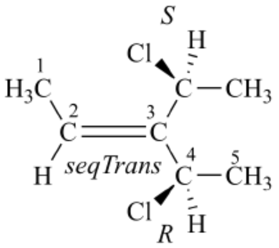
Example 4:


5
4
3
Y
6
1
2
6
2
X
S
Br
H
Y =
C
CH$_3$
R
H
Br
X =
C
CH$_3$

(1^1*m*)-1^2-[(1*R*)-1-bromoethyl]-1^6-[(1*S*)-1-bromoethyl]-1,4(1,4)-dibenzenacyclohexaphane (PIN)
(1^1*s*$_p$)-1^2-[(1*R*)-1-bromoethyl]-1^6-[(1*S*)-1-bromoethyl]-1,4(1,4)-dibenzenacyclohexaphane

Explanation: The configurations for 'X' and 'Y' are determined by applying Sequence Rule **1**. The configuration '*m*' or '*s*$_p$' at 'C-11' is determined in accordance with the methodology described in P-92.1.2.1.3 and P-92.1.2.2.2 (see also P-93.5.5.1).

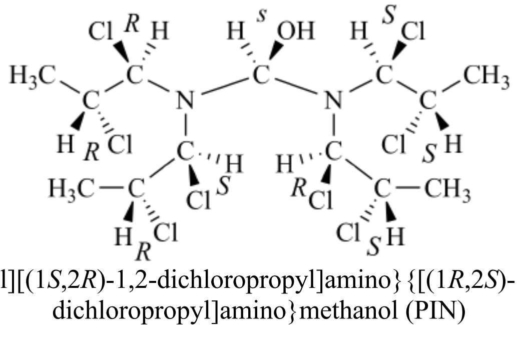
Example 5:


S
Cl
H
1
H$_3$C
C—CH$_3$
2
3
C═C
H
seqTrans
4
5
C—CH$_3$
Cl
R
H

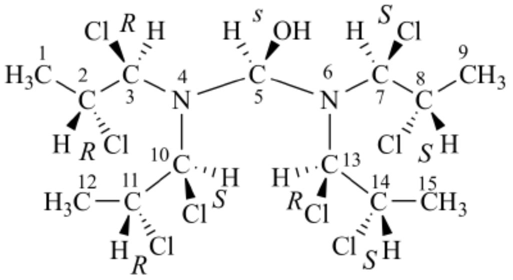
(2*seqTrans*,4*R*)-4-chloro-3-[(1*S*)-1-chloroethyl]pent-2-ene (PIN)

Explanation: 'The configurations at 'C-4' and for the side chain are determined by applying Sequence Rule **1**. The configuration '*seqTrans*' is determined in accordance with the methodology described in P-92.4.1, priority being assigned to '*R*' over '*S*' on the same side of the reference plane.

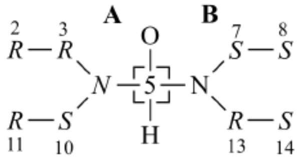
Example 6:


Cl
R
H
H
s
OH
H
S
Cl
H$_3$C
C
N
C
N
C
CH$_3$
C
C
H
R
Cl
Cl
S
H
C
H
H
C
H$_3$C—C
Cl
S
R
Cl
C—CH$_3$
H
R
Cl
Cl
S
H

(*s*)-{[(1*R*,2*R*)-1,2-dichloropropyl][(1*S*,2*R*)-1,2-dichloropropyl]amino}{[(1*R*,2*S*)-1,2-dichloropropyl][(1*S*,2*S*)-1,2-dichloropropyl]amino}methanol (PIN)



arbitrary numbering used in the construction of theigraph for at ‘C-5’



reference descriptor

reference descriptor

pairs of descriptors

R	***S***	***R***	***S***
R, 3 → *l*	*S*, 10 → *l*	*R*, 13 → *l*	*S*, 7 → *l*
R, 10 → *u*	*S*, 3 → *u*	*R*, 7 → *u*	*S*, 13 → *u*
R, 2 → *l*	*S*, 11 → *u*	*R*, 14 → *u*	*S*, 8 → *l*
R, 11 → *l*	*S*, 2 → *u*	*R*, 8 → *u*	*S*, 14 → *l*

$$\begin{array}{ccc} R\ lull & & R\ luuu \\ & = & \\ S\ luuu & & S\ lull \\ \mathbf{A} & = & \mathbf{B} \end{array}$$

Explanation: First, the molecule is arbitrarily renumbered as above: Then, the ligands are analyzed by Sequence Rule **4b** and Sequence Rule **1** is applied, leading to the specification of eight chirality centers ‘C-2’, ‘C-3’, ‘C-7’, ‘C-8’, ‘C-10’, ‘C-11’, ‘C-13’, ‘C-14’ as shown above. For the specification of the configuration at ‘C-5’, Sequence Rule **4b** is applied in accordance with the following digraph and methodology described in P-92.5.2.1. No decision is reached because ‘branch A’ = ‘branch B’, as indicated by the result of the following analysis thus necessitating the application of Sequence Rule **5**.

Ranking of ligands by Sequence Rule **5**:

By application of Sequence Rule **5** using the same digraph a decision is reached after the following analysis. As in the set of highest ranked nodes both descriptors ‘*R*’ and ‘*S*’ are present, both of them must be used as reference descriptors.

When Sequence Rule **5**, ‘*R*’ precedes ‘*S*’, is applied to the first sphere of descriptors (those directly bonded to N), in ’branch A’ node 3 ranks higher than node 10; in ‘branch B’ node 13 ranks higher than node 7. At this level, no difference is noted. At the next level, where descriptors ‘2’ and ‘11’ and ‘8’ and ‘14’ are located, the highest ranking node 2 is ‘*R*’ in ‘branch A’ and the highest ranking node 14 is ‘*S*’ in ‘branch B’; this is the first difference noticed permitting the ranking of ‘branch A’ over ‘branch B’; thus the configuration ‘*s*’ is assigned to ‘C-5’.

Branch A	Branch B	
3-‘*R*’	13-‘*R*’	
10-‘*S*’	7-‘*S*’	
2-‘*R*’	14-‘*S*’	(first difference encountered)
11-‘*R*’	8-‘*S*’	

Branch A > Branch B

P-93 CONFIGURATION SPECIFICATION

P-93.0 Introduction
P-93.1 General aspects of configuration specification
P-93.2 Tetrahedral configuration of elements other than carbon
P-93.3 Nontetrahedral configuration
P-93.4 Configuration specification of acyclic organic compounds
P-93.5 Configuration specification of cyclic organic compounds
P-93.6 Compounds composed of rings and chains

P-93.0 INTRODUCTION

Different systems are used to describe the configuration of acyclic and cyclic compounds. In Sections P-92, the various CIP stereodescriptors were described in accordance with different types of configuration. This Section describes these various systems and the selection of preferred descriptors to denote the configuration in preferred names. They are applied on the basis of the parent structures, i.e., acyclic or cyclic, along with the non-CIP stereodescriptors that are recommended for general nomenclature.

P-93.1 GENERAL ASPECTS OF CONFIGURATION SPECIFICATION

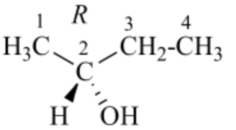
In the context of stereochemistry, the term 'configuration' is restricted to the arrangements of atoms of a molecular entity in space that distinguishes 'stereoisomers', the isomerism between which is not due to conformational differences. 'Conformation' is the spatial arrangement of the atoms affording distinction between stereoisomers which can be interconverted by rotation about formally single bonds. Configuration is discussed in this section, P-93; conformation is discussed in section P-94.

P-93.1.1 Absolute configuration
P-93.1.2 Relative configuration
P-93.1.3 Racemates
P-93.1.4 The descriptor '*ambo*'

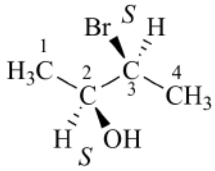
P-93.1.1 Absolute configuration

The 'absolute configuration' is the spatial arrangement of the atoms of a chiral molecular entity. It corresponds to a graphical representation and is described by stereodescriptors such as '*R*', '*S*', '*r*', '*s*', '*M*', or '*P*', as shown in Section P-92.

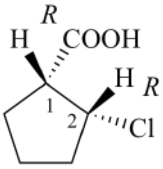
Examples:



(2*R*)-butan-2-ol (PIN)



(2*S*,3*S*)-3-bromobutan-2-ol (PIN)

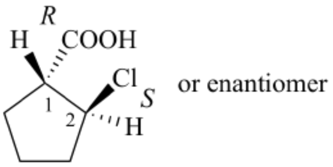


(1*R*,2*R*)-2-chlorocyclopentane-1-carboxylic acid (PIN)

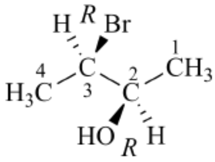
P-93.1.2 Relative configuration

P-93.1.2.1 The 'relative configuration' is the configuration of any stereogenic (asymmetric) unit with respect to any other stereogenic unit contained within the same molecular entity. Relative configuration denoting diastereoisomers may be denoted by using the prefix '*rel*' which is cited at the front of the name of one enantiomer where the configurational descriptors '*R*', '*S*', '*M*', '*P*', etc. have been used. This prefix '*rel*' with plain stereodescriptors is preferred in preferred IUPAC names to the 'starred' stereodescriptors '*R**', '*S**', '*M**', '*P**', etc. that may be used in general nomenclature. It is to be noted that the prefix '*rel*' indicates the configuration of the entire molecule. The structure of one enantiomer followed by the mention 'or enantiomer' is used to depict relative configuration. When relative configuration is described, the stereodescriptor, such as '*R*' or '*R**', is cited for the stereogenic center having the lowest locant.

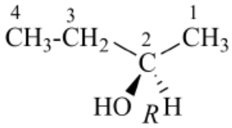
Examples:



rel-(1*R*,2*S*)-2-chlorocyclopentane-1-carboxylic acid (PIN)
(1*R**,2*S**)-2-chlorocyclopentane-1-carboxylic acid
trans-2-chlorocyclopentane-1-carboxylic acid
(see P-93.5.1.2 for use of the non-CIP stereodescriptor '*trans*')
[not *rel*-(1*S*,2*R*)-2-chlorocyclopentane-1-carboxylic acid]
[not (1*S**,2*R**)-2-chlorocyclopentane-1-carboxylic acid]


or enantiomer

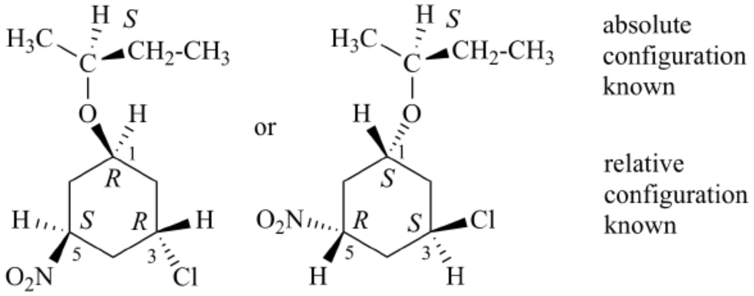
rel-(2*R*,3*R*)-3-bromobutan-2-ol (PIN)
(2*R**,3*R**)-3-bromobutan-2-ol


or enantiomer

rel-(2*R*)-butan-2-ol (PIN)
(2*R**)-butan-2-ol

P-93.1.2.2 In compounds containing chirality centers with known absolute configurations and a stereochemically unrelated set of chirality centers with known relative configuration, the '*R**' and '*S**' descriptors must be used to designate the latter. The prefix '*rel*' cannot be used as it applies to the entire molecule.

Example:



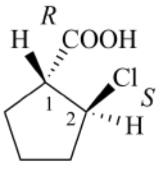
(1*R**,3*R**,5*S**)-1-{[(2*S*)-butan-2-yl]oxy}-3-chloro-5-nitrocyclohexane (PIN)

P-93.1.3 Racemates

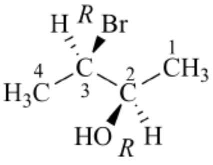
A racemate is an equimolecular mixture of a pair of enantiomers. It does not exhibit optical activity. Racemates may be denoted by using the prefix '*rac*' cited at the front of the name of one enantiomer where the configurational descriptors '*R*', '*S*', '*M*', '*P*', etc. have been used. This prefix '*rac*' with plain stereodescriptors is preferred in preferred IUPAC names to the stereodescriptors such as '*RS*', '*SR*', etc. that may be used in general nomenclature. It is to be noted that the prefix '*rac*' indicates the configuration of the entire molecule.

The structure of one enantiomer followed by the mention 'and enantiomer' is used to depict racemates. When a racemate is described, the stereodescriptor, such as '*R*' or '*RS*', is cited for the chirality center having the lowest locant.

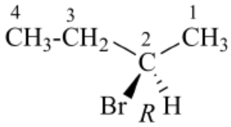
Examples:


and enantiomer

rac-(1*R*,2*S*)-2-chlorocyclopentane-1-carboxylic acid (PIN)
(1*RS*,2*SR*)-2-chlorocyclopentane-1-carboxylic acid


and enantiomer

rac-(2*R*,3*R*)-3-bromobutan-2-ol (PIN)
(2*RS*,3*RS*)-3-bromobutan-2-ol

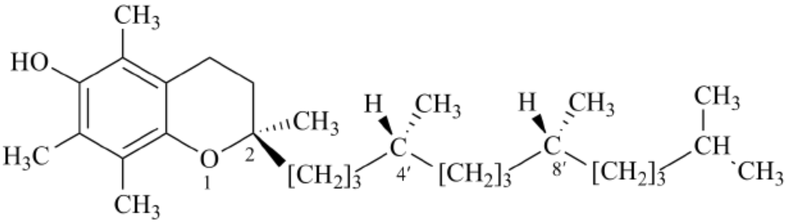

and enantiomer

rac-(2*R*)-2-bromobutane (PIN)
(2*RS*)-2-bromobutane
(±)-2-bromobutane

P-93.1.4 The descriptor ‘*ambo*’

Formation of diastereoisomers by reaction at a nonstereogenic center of a chiral molecule or the reaction of a chiral compound with a racemic compound will not normally give a 50-50 mixture. To indicate this situation, the prefix ‘*ambo*’ is used (see also P-103.3.4).

Example:



plus a proportion of the epimer at C-2
2-*ambo*-(2*R*,4′*R*,8′*R*)-α-tocopherol (refs. 37, 44)
2-*ambo*-(2*R*)-2,5,7,8-tetramethyl-2-[(4*R*,8*R*)-4,8,12-trimethyltridecyl]-3,4-dihydro-2*H*-1-benzopyran-6-ol

P-93.2 TETRAHEDRAL CONFIGURATION OF ELEMENTS OTHER THAN CARBON

P-93.2.0 Introduction
P-93.2.1 General methodology
P-93.2.2 Azanium (ammonium) and phosphanium (phosphonium) compounds
P-93.2.3 Amine oxides and phosphane oxides
P-93.2.4 Phosphates, phosphonates, and related compounds
P-93.2.5 Sulfates, sulfonates, and related compounds
P-93.2.6 Compounds of Group 14 (other than carbon compounds)

P-93.2.0 Introduction

The CIP priority system described for stereogenic carbon centers is extended to any atom having four ligands tetrahedrally arranged. Many examples are illustrated in this section.

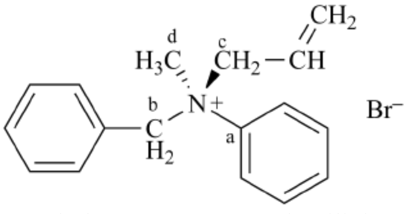
P-93.2.1 General methodology

The absolute configuration of any chirality center with four ligands tetrahedrally arranged is described by ‘*R*’ and ‘*S*’ stereodescriptors; the absolute configuration of pseudoasymmetric centers is described by ‘*r*’ and ‘*s*’. The assignment of these descriptors is the same as for carbon compounds. Numerical locants are used before stereodescriptors, but letter locants such as ‘*N*’, ‘*O*’ or ‘*S*’ are not. To avoid uncertainty in preferred IUPAC names, in the absence of any reference locant in the name, the name of the compound containing the stereogenic unit whose central atom is B, S, Se, Te, N, P, As, Sb, Bi is written within appropriate nesting marks. In general nomenclature, locants and specific nesting can be omitted.

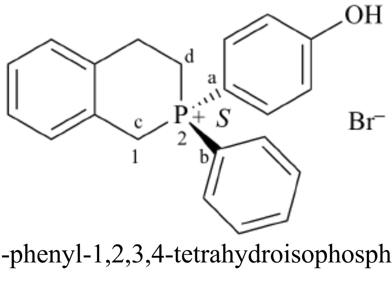
P-93.2.2 Azanium (ammonium) and phosphanium (phosphonium) compounds

The four different ligands are considered in priority order ‘a’ > ‘b’ > ‘c’ > ‘d’ in the manner described in P-92.2. Stereodescriptors are cited as indicated in P-91.2.

Examples:



(*R*)-*N*-benzyl-*N*-methyl-*N*-(prop-2-en-1-yl)anilinium bromide (PIN)
(*R*)-*N*-benzyl-*N*-methyl-*N*-(prop-2-en-1-yl)benzenaminium bromide
(*R*)-benzyl(methyl)(phenyl)(prop-2-en-1-yl)azanium bromide
(*R*)-benzyl(methyl)(phenyl)(prop-2-en-1-yl)ammonium bromide



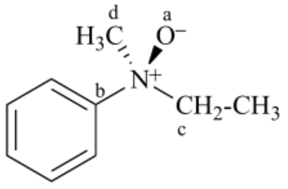
(2*S*)-2-(4-hydroxyphenyl)-2-phenyl-1,2,3,4-tetrahydroisophosphinolin-2-ium bromide (PIN)

Arsanium, stibanium, and bismuthanium salts are treated in the same manner as phosphorus centered cations.

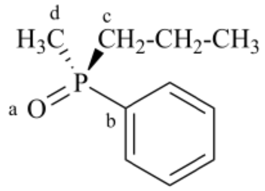
P-93.2.3 Amine oxides and phosphane oxides

With chiral amine oxides and phosphane oxides the oxygen atom is treated as the fourth atom. The nature of the bonding to this oxygen atom is not relevant.

Examples:



(*S*)-*N*-ethyl-*N*-methylaniline *N*-oxide (PIN; see P-74.2.1.2)
(*S*)-[ethyl(methylbenzenaminiumyl]oxidanide
[(*S*)-ethyl(methyl)(phenyl)azaniumyl]oxidanide

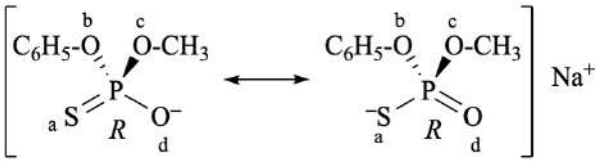


(*S*)-methyl(phenyl)(propyl)-λ^5-phosphanone (PIN; see P-74.2.1.4)
(*S*)-methyl(phenyl)(propyl)phosphane oxide

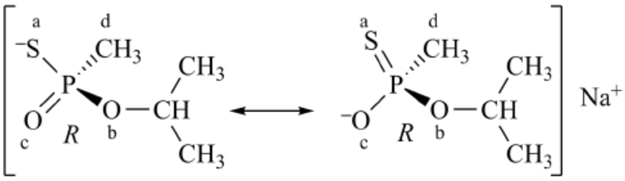
P-93.2.4 Phosphates, phosphonates, and related compounds

The ‘P=O’ bond, as conventionally written in phosphates, phosphonates and related compounds, is considered as a single bond, as there are already four atoms or groups in the tetrahedral configuration. Similarly, the formal arrangement of charges is not considered when determining the configuration of a chiral molecule. As the stereodescriptors ‘*R*’ and ‘*S*’ describe the entire structure, either a salt or an ester, the full name is placed in parentheses to denote the global configuration.

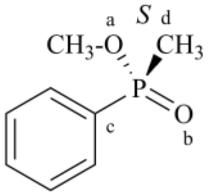
Examples:



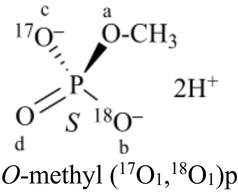
sodium (*R*)-(*O*-methyl *O*-phenyl phosphorothioate) (PIN)



sodium (*R*)-(*O*-propan-2-yl methylphosphonothioate) (PIN)
sodium (*R*)-[*O*-(1-methylethyl) methylphosphonothioate]



methyl (*S*)-[methyl(phenyl)phosphinate] (PIN)

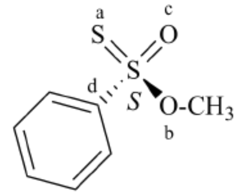


dihydrogen (*S*)-[*O*-methyl (${}^{17}\text{O}_1$,${}^{18}\text{O}_1$)phosphate] (PIN)

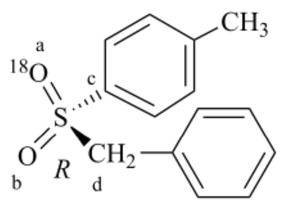
P-93.2.5 Sulfates, sulfonates, and related compounds

Sulfates, sulfonates and related anions are treated in the same way as phosphate anions (see P-93.2.4). Selenates, selenonates, tellurates, telluronates and related compounds are treated like sulfates, sulfonates and related compounds. Sulfoxides are discussed in P-93.3.3.2.

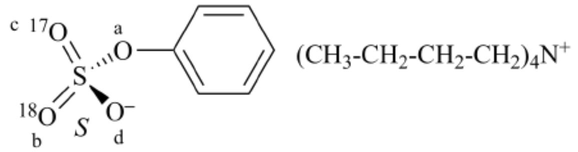
Examples:



O-methyl (*S*)-(benzenesulfonothioate) (PIN)



1-methyl-4-[(*R*)-phenyl($^{18}O_1$)methanesulfonyl]benzene (PIN)

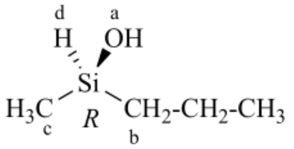


N,*N*,*N*-tributylbutan-1-aminium (*S*)-[*O*-phenyl ($^{17}O_1$,$^{18}O_1$)sulfate] (PIN; see also P-83.1.2.2)
tetrabutylammonium (*S*)-[*O*-phenyl ($^{17}O_1$,$^{18}O_1$)sulfate]
tetrabutylazanium (*S*)-[*O*-phenyl ($^{17}O_1$,$^{18}O_1$)sulfate]

P-93.2.6 Compounds of Group 14 (other than carbon compounds)

Chiral silanes, germanes, stannanes, and plumbanes are treated in the same way as carbon compounds.

Example:



(*R*)-methyl(propyl)silanol (PIN)

P-93.3 NONTETRAHEDRAL CONFIGURATION

P-93.3.1 General methodology
P-93.3.2 Polyhedral symbols
P-93.3.3 Configuration index and priority number
P-93.3.4 Chirality symbols

P-93.3.1 General methodology

When an atom is attached to three, four, five, or six ligands (atoms or groups) a number of geometrical configurations are possible. In general, there will be some distortion from the idealized geometry of the regular solid due to differences between the atoms involved. Thus with five attached ligands they may be arranged as a trigonal bipyramid or square pyramid and with six as an octahedron or trigonal prism (which is much less common). The notation described below for these systems is described in the IUPAC rules for inorganic coordination nomenclature (IR-9.3, ref. 12). Details of the geometry of systems with a coordination greater than six will also be found in ref. 12.

Stereodescriptors for nontetrahedral configurations are composed of three parts.

(1) A symbol indicating overall geometry called the ‘polyhedral symbol’;

(2) A symbol called the ‘configuration index’ that describes the configuration of ligands around the central atom;

(3) A symbol indicating the ‘absolute configuration’ associated with the central atom called the ‘chirality symbol’.

The three parts of the stereodescriptor are enclosed in parentheses and separated from each other by hyphens and cited at the front of the name separated from it by a hyphen.

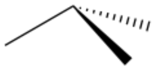
P-93.3.2 Polyhedral symbols

The polyhedral symbol takes the form of an abbreviation of the name of the closest idealized geometry (italic upper case letters) and a number indicating how many ligands are attached (see Rule IR-9.3.2.1, ref. 12). Table 9.1 gives the symbols for the most frequently encountered polyhedra related to structures of organic compounds. The configuration of molecules containing a tetrahedral center has been discussed above in Section P-92.

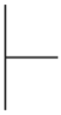
The abbreviation for the idealized polyhedron and the number of attached atoms or groups are separated by a hyphen and enclosed in parentheses in front of the name of the compound, if no further information is required.

Table 9.1 Commonly encountered polyhedral symbols in organic compounds

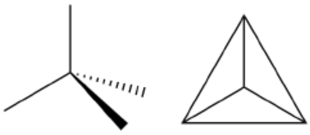
Idealized geometry	Attached atoms or groups	Polyhedral symbol
trigonal pyramid	3	*TPY*-3
T-shape	3	*TS*-3 (ref. 12)
tetrahedron	4	*T*-4
square planar	4	*SP*-4
see-saw	4	*SS*-4 (ref. 12)
trigonal bipyramid	5	*TBPY*-5
square pyramid	5	*SPY*-5
octahedron	6	*OC*-6



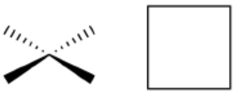
TPY-3



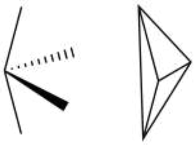
TS-3



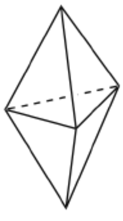
T-4



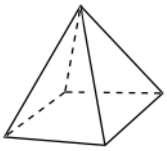
SP-4



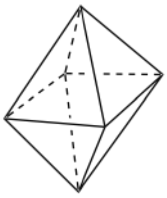
SS-4



TBPY-5

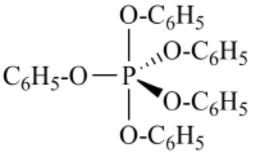


SPY-5

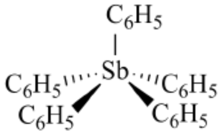


OC-6

Examples:



(*TBPY*-5)-pentaphenoxy-λ^5-phosphane (PIN)



(*SPY*-5)-pentaphenyl-λ^5-stibane (PIN)

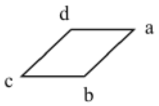
P-93.3.3 Configuration index and priority rules

P-93.3.3.1 General methodology
P-93.3.3.2 Trigonal pyramid
P-93.3.3.3 T-shape systems
P-93.3.3.4 See-saw systems
P-93.3.3.5 Trigonal bipyramid
P-93.3.3.6 Square pyramid
P-93.3.3.7 Octahedron

P-93.3.3.1 General methodology

The configuration index is a series of numbers to identify where each atom or group is located (see Rule IR-9.3.3.2, ref. 12). It is based on the CIP priority order (see P-92) of the atoms attached. The atom or atoms with highest priority are given priority number one '1'; the next priority number two '2', and so on. In the examples below, structures are denoted by locants. They are also denoted by circled numbers that are the priority numbers used in the application of the CIP system. In addition to the standard CIP Sequence Rules **1** and **2**, three additional rules are needed:

(a) The '*trans*-maximum-difference' of priority (see IR-9.3.3.3, ref. 12). Between atoms with the same priority number, high priority is assigned to the atom which is *trans* (opposite) to the atom having the lowest priority number. In the following planar structure, 'a and c' (and 'b and d') are '*trans*':



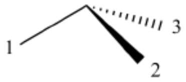
(b) The priming convention (see IR-9.3.5.3, ref. 12). When there are two (or three) identical rings present, the priority numbers of one of them are primed (and the third double primed).

(c) Unprimed priority numbers are preferred to primed priority numbers. In coordination nomenclature rings are di- and polydentate ligands.

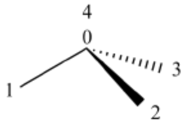
Each idealized geometry has its own rules for assignment of the configuration index.

P-93.3.3.2 Trigonal pyramid

The configuration of molecules containing a trigonal pyramidal center (*TPY*-3) is described in a similar way to that of tetrahedral centers (T-4) described above in P-92 (see IR-9.3.4.3, ref. 12). The tetrahedral configuration is achieved by adding a phantom atom (0) to the central atom perpendicular to the base of the pyramid. No configuration index is used with the '*TPY*-3' symbol. Priority numbers are '1 > 2 > 3 > 4'.



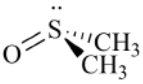
TPY-3



(*T*-4) (a phantom atom ‘0’ is shown)

Traditionally, sulfoxides have been considered as a tetrahedral system composed of a central atom, ligands, and a lone pair of electrons (or phantom atom). No polyhedral symbol is used.

Example:



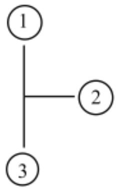
(methanesulfinyl)methane (PIN)
[not (*T*-4)-(methanesulfinyl)methane;
the symbol (*T*-4) is not used in the names of organic compounds]

P-93.3.3.3 T-shape systems

The configuration index of the T-shape configuratio

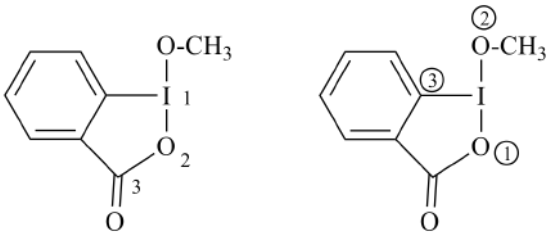
n follows the polyhedral symbol, *TS*-3, and consist of a single digit, the priority number of the atom or substituent group on the stem of the ‘T’ (as opposed to the cross piece of the ‘T’) (see IR-9.3.3.7, ref. 12).

Example:



(*TS*-3-2)

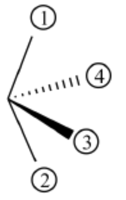
Example:



(*TS*-3-3)-1-methoxy-1λ^3,2-benziodoxol-3(1*H*)-one (PIN)
[not (*TBPY*-3)-1-methoxy-1λ^3,2-benziodoxol-3(1*H*)-one; see P-93.3.3.5.1]

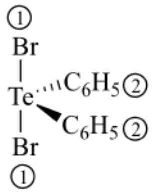
P-93.3.3.4 See-saw systems

The configuration index of a see-saw system consists of the priority numbers indicating the two atoms or groups separated by the largest angle (see IR-9.3.3.8, ref. 12).



(*SS*-4-12)

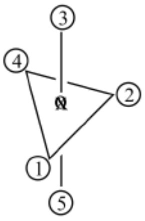
Example:



(*SS*-4-11)-dibromodiphenyl-λ^4-tellurane (PIN)
[not *TBPY*-4-dibromodiphenyl-λ^4-tellurane (see P-93.3.3.5.1)]

P-93.3.3.5 Trigonal bipyramid

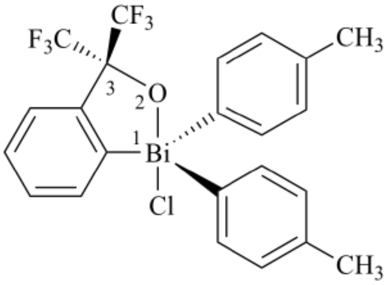
P-93.3.3.5.1 The configuration index of a trigonal bipyramid (see Rule IR-9.3.3.6, ref 12) consists of the priority numbers of the two apical atoms (lower number first if different), representing the reference axis of the system. Priority numbers are: '1 > 2 > 3 > 4 > 5'.



(*TBPY*-5-35)

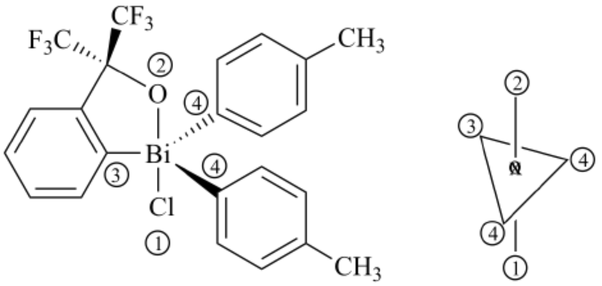
The polyhedral symbol and configuration index, separated by a hyphen, are enclosed in parentheses and placed at the front of the name of the compound, if no further information is required.

Example:



(*TBPY*-5-12)-1-chloro-1,1-bis(4-methylphenyl)-3,3-bis(trifluoromethyl)-1,3-dihydro-2,1λ^5-benzoxabismole (PIN)

Explanation:

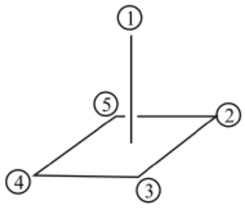


P-93.3.3.5.2 The trigonal bipyramid system has been extended to central atoms substituted by four ligands and one lone pair of electrons, and by three ligands and two lone pairs of electrons (see SP-9.2, ref. 8).

When one lone pair is present, the polyhedral symbol is '*TBPY*-4'; the symbol is '*TBPY*-3' when two lone pairs of electrons are present. This system is no longer recommended. Instead, in preferred IUPAC names, the polyhedral symbol '*SS*' is used in place of '*TBPY*-4' for see-saw systems (see P-93.3.3.4); similarly the symbol '*TS*-3' is used in place of '*TBPY*-3' for T-shape systems (see P-93.3.3.3).

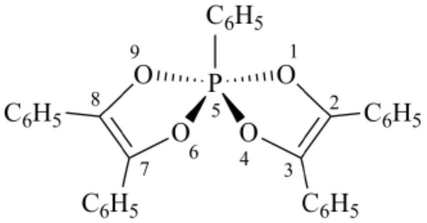
P-93.3.3.6 Square pyramid

The configuration index of a square pyramid (see Rule IR-9.3.3.5, ref. 12) is given by two numbers. The first is the priority number of the apical atom and the second is the priority number of the atom *trans* (opposite) with reference to the atom having the highest priority (lowest priority number) in the base of the pyramid. If necessary, the rule of the '*trans*-maximum difference of priority numbers' is applied (see Rule IR- 9.3.3.3, ref. 12). The reference axis corresponds to the bond to the apical ligand. The polyhedral symbol and configuration index, separated by a hyphen, are enclosed in parentheses and cited in front of the name of the compound, if no further information is required. For the ranking order '1 > 2 > 3 > 4 > 5', the following configuration is denoted by the configuration index '14'.



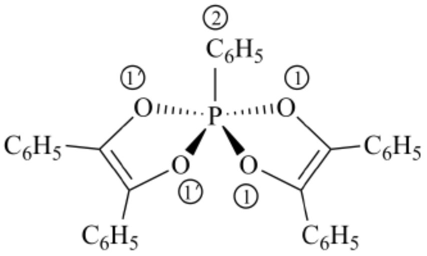
(*SPY*-5-14)

Example 1:

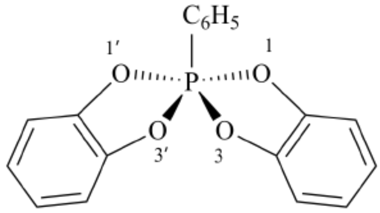

C_6H_5
9
1
O
P
O
8
2
C_6H_5
5
C_6H_5
O
O
6
4
7
3
C_6H_5
C_6H_5

(*SPY*-5-21′)-2,3,5,7,8-pentaphenyl-1,4,6,9-tetraoxa-5λ^5-phosphaspiro[4.4]nona-2,7-diene (PIN)

Explanation:

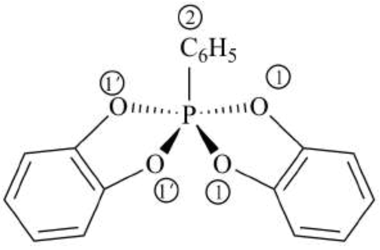

②
C_6H_5
①′
①
O
P
O
C_6H_5
C_6H_5
O
O
①′
①
C_6H_5
C_6H_5

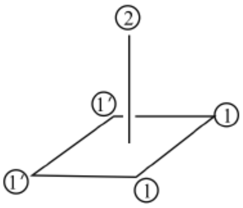
Example 2:


C_6H_5
1′
1
O
P
O
O
O
3′
3

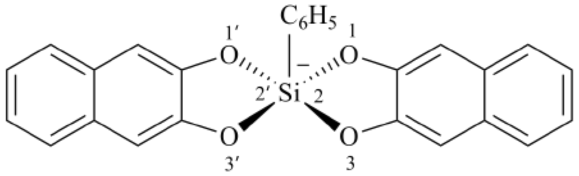
(*SPY*-5-21′)-2-phenyl-2*H*-2λ^5,2′-spirobi[[1,3,2]benzodioxaphosphole] (PIN)

Explanation:


②
C_6H_5
①′
①
O
P
O
O
O
①′
①

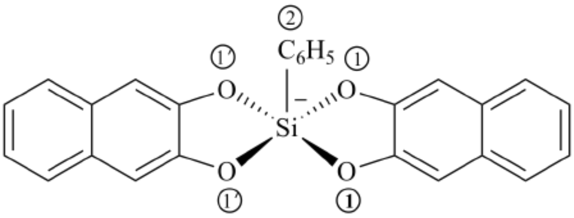


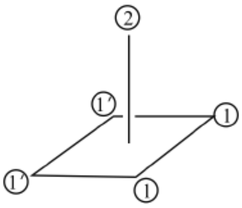
Example 3:


C_6H_5
1′
1
O
−
O
2′
Si
2
O
O
3′
3

(*SPY*-5-21′)-2-phenyl-2*H*-2,2′-spirobi[naphtho[2,3-*d*][1,3,2]dioxasilol]-2-uide (PIN)

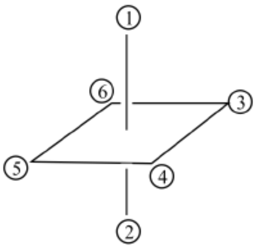
Explanation:





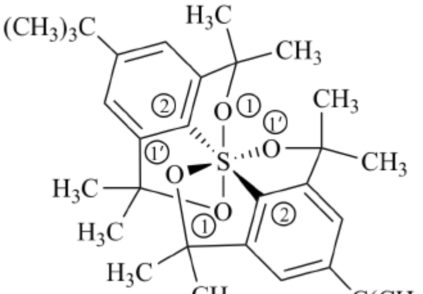
P-93.3.3.7 Octahedron

The configuration index of an octahedron (see Rule IR-9.3.3.4, ref. 12) is given by two numbers. The first is the priority number of the atom '*trans*' (opposite) to the atom of highest priority (lowest priority number). This defines the reference axis. The second number is the priority number of the atom '*trans*' (opposite) the atom of highest priority (lowest priority number) in the plane perpendicular to the reference axis. If necessary, the principle of the '*trans*-maximum-difference' of priority numbers is applied. The polyhedral symbol and configuration index, separated by a hyphen, are enclosed in parentheses and cited in front of the name of the compound, if no further information is needed. For the order of priority '1 > 2 > 3 > 4 > 5 > 6', the configuration index is '25', as illustrated below.



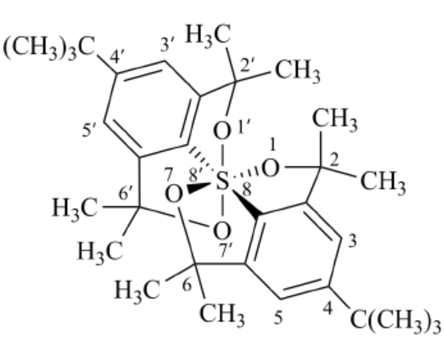
(*OC*-6-25)

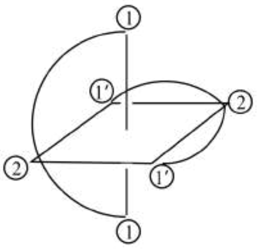
Example:



(*OC*-6-11′)-4,4′-di-*tert*-butyl-2,2,2′,2′,6,6,6′,6′-octamethyl-2*H*,2′*H*,6*H*,6′*H*-8λ^6,8′-spirobi[[1,2]oxathiolo[4,3,2-*hi*][2,1]benzoxathiole] (PIN)

Explanation:





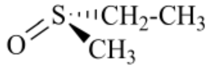
P-93.3.4 Chirality symbols

The chirality symbols '*A*' and '*C*' are used to indicate the absolute configuration of compounds described by a polyhedral symbol and a configuration index, with the exception of trigonal pyramidal polyhedra that are described by '*R*' and '*S*' stereodescriptors (see P-93.3.4.1) and tetrahedral configuration that is described in P-92.1.1.

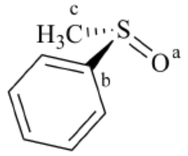
P-93.3.4.1 The chirality symbols '*R/S* '.

The stereodescriptors '*R*' and '*S*' (as defined in P-92.2) are used to indicate the absolute configuration of a trigonal pyramidal system discussed in P-93.3.3.2 (see Rule IR-9.3.4.3, ref. 12). A phantom atom of low priority, and not a pair of electrons, is used to create the tetrahedral configuration permitting the use of '*R/S*' stereodescriptors in the manner described for tetrahedral stereogenic centers.

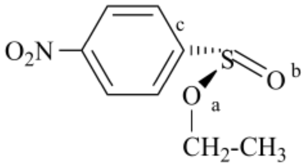
Examples:



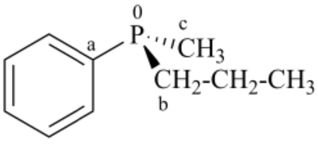
(*S*)-(methanesulfinyl)ethane (PIN)



(*S*)-(methanesulfinyl)benzene (PIN)



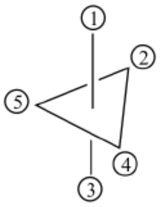
ethyl (*R*)-4-nitrobenzene-1-sulfinate (PIN)



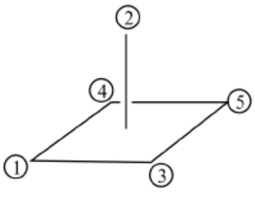
(*R*)-methyl(phenyl)(propyl)phosphane (PIN)
(a phantom atom, '0', is shown on the phosphorus atom)

P-93.3.4.2 The chirality symbols '*A*' and '*C*'

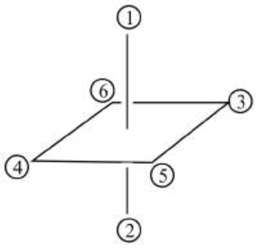
P-93.3.4.2.1 The atoms in the plane perpendicular to the reference axis are viewed from the side with the atom or group of highest priority (lowest priority number) on the reference axis. If the direction from the atom in this plane with highest priority (lowest priority number) to the atom with the next higher priority is clockwise the chirality symbol is '*C*', if anticlockwise '*A*'. The term 'anticlockwise' is also called 'counterclockwise'. The polyhedral symbol, configuration index, and chirality symbol, each separated by a hyphen, are enclosed in parentheses and cited in front of the name of the compound (see Rule IR-9.3.4.4, ref. 12). The order of priority '1 > 2 > 3 > 4 > 5 > 6' for the trigonal bipyramid, the square pyramid, and the octahedral configurations are illustrated below:



TBPY-5-13-*C*

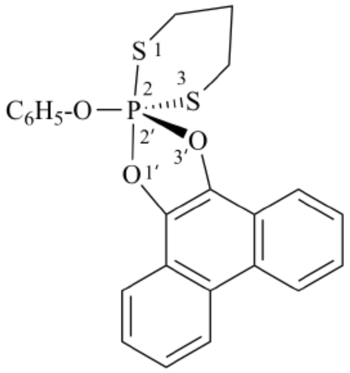


SPY-5-25-*A*



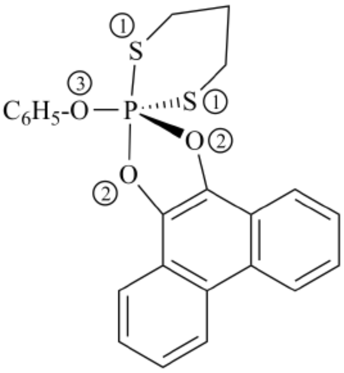
OC-6-24-*C*

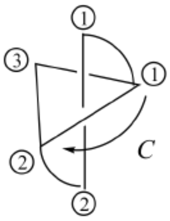
Example 1:


S 1
2
3
S
C_6H_5-O
P
2′
O
3′
O 1′

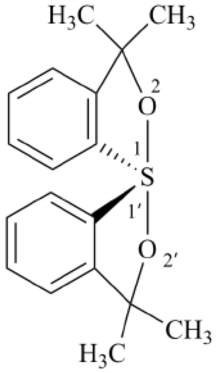
(*TBPY*-5-12-*C*)-2-phenoxy-2*H*-2λ^5-spiro[[1,3,2]dithiaphosphinane-2,2′-phenanthro[9,10-*d*][1,3,2]dioxaphosphole] (PIN)

Explanation:


①
S
③
C_6H_5-O
P
S ①
O ②
O
②

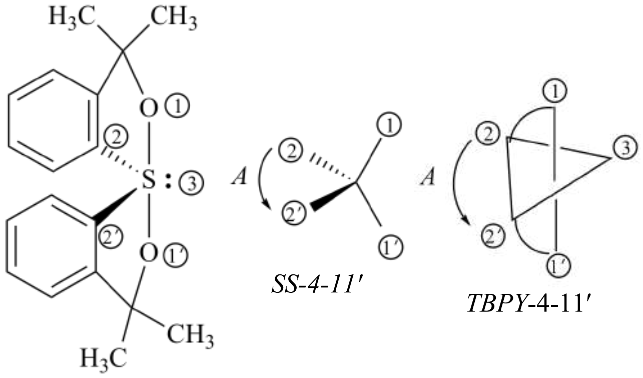


Example 2:


H_3C
CH_3
O 2
1
S
1′
O 2′
CH_3
H_3C

(*SS*-4-11′-*A*)-3,3,3′,3′-tetramethyl-3*H*,3′*H*-1λ^4,1′-spirobi[[2,1]benzoxathiole] (PIN)
[not (*TBPY*-4-11′-*A*)-3,3,3′,3′-tetramethyl-3*H*,3′*H*-1λ^4,1′-spirobi[[2,1]benzoxathiole]]

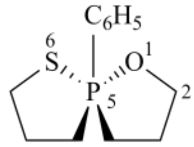
Explanation:


H₃C
CH₃
O ①
②
S : ③
②′
O ①′
CH₃
H₃C
A
①
②
②′
①′
A
①
②
③
②′
①′

SS-4-11′

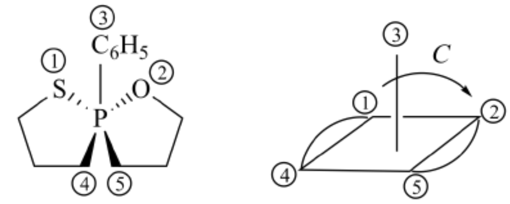
TBPY-4-11′

Example 3:

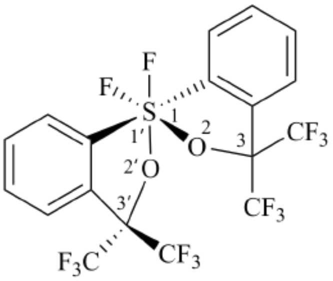

C₆H₅
6
S
O
1
P
5
2

(*SPY*-5-35-*C*)-5-phenyl-1-oxa-6-thia-5λ^5-phosphaspiro[4.4]nonane (PIN)

Explanation:

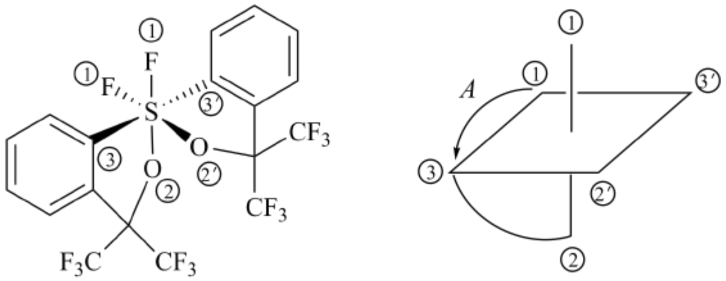

③
C₆H₅
①
S
O
②
P
④
⑤
③
C
①
②
④
⑤

Example 4:


F
F
S
1
1′
2
O
3
CF₃
2′
O
3′
CF₃
F₃C
CF₃

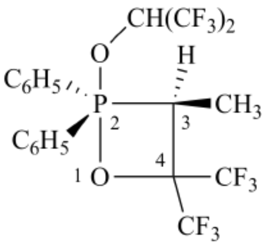
(*OC*-6-22′-*A*)-1,1-difluoro-3,3,3′,3′-tetrakis(trifluoromethyl)-1,3′-dihydro-3*H*-1λ^6,1′-spirobi[[2,1]benzoxathiole] (PIN)

Explanation:


①
F
①
F
S
③′
③
O
②′
CF₃
O
②
CF₃
F₃C
CF₃
①
A
①
③′
③
②′
②

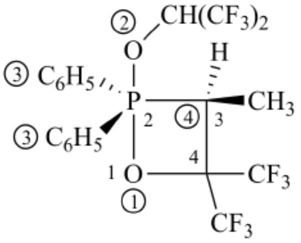
P-93.3.4.2.2 When necessary, the locant of the chirality center is included in front of the polyhedral descriptor, and other chirality centers are specified in accordance with the increasing value of locants as indicated in P-91.3; brackets enclose the complete descriptor denoting the overall geometry of the molecule.

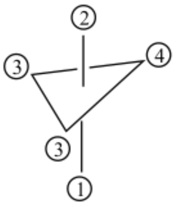
Example:



[2(*TBPY*-5-12),3*S*]-2-[(1,1,1,3,3,3-hexafluoropropan-2-yl)oxy]-3-methyl-2,2-diphenyl-4,4-bis(trifluoromethyl)-1,2λ^5-oxaphosphetane (PIN)

Explanation:





P-93.4 CONFIGURATION SPECIFICATION OF ACYCLIC ORGANIC COMPOUNDS

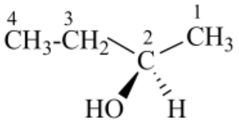
This section illustrates the CIP priority system as the preferred system of specification of configuration and describes other systems that are used in substitutive nomenclature. Preferred names are formed in accordance with the principles, rules, and convention described in Chapters P-1 through P-8. Numbering of compounds is established by applying rules described in P-14.4, especially when the final choice depends on the presence of stereodescriptors. Stereodescriptors are added to the names as indicated in P-91.3.

P-93.4.1 Specification of stereogenic centers
P-93.4.2 Specification of configuration for double bonds

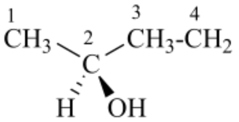
P-93.4.1 Specification of stereogenic centers

P-93.4.1.1 The presence of one stereogenic center is denoted by the stereodescriptors '*R*' and '*S*', as described in P-92.2. Stereodescriptors are preceded by a locant when the stereogenic center needs to be described by a locant. When no locant is required in the name of the chiral compound, no locant is necessary before the stereodescriptor. The symbol (±), (+) or (–) may be used in general nomenclature.

Examples:



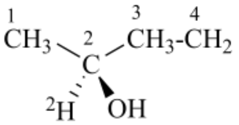
(2*R*)-butan-2-ol (PIN)



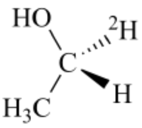
(2*S*)-butan-2-ol (PIN)

When required, either Sequence Rule **1** alone or both Sequence Rules **1** and **2** are applied to specify the configuration of isotopically modified compounds as illustrated below (see also P-92.3). When inserted into the name at the same place as isotopic descriptors, the stereochemical affixes are cited first.

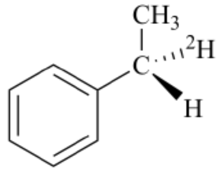
Examples:



(2*S*)-(2-^{2}H)butan-2-ol (PIN)



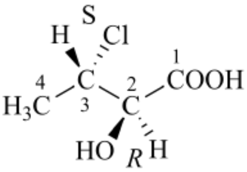
(1*R*)-(1-^{2}H$_1$)ethan-1-ol (PIN)



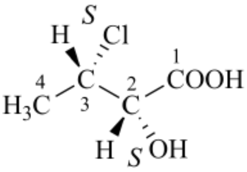
[(1*S*)-(1-$^2H_1$)ethyl]benzene (PIN)

P-93.4.1.2 When, in a parent structure, two or more stereodescriptors, '*R*' and/or '*S*', are required to describe a single structure, they are placed at the front of the name, enclosed in parentheses followed by a hyphen, and cited according to the ascending order of their corresponding locants, regardless of the kind of descriptor. Many examples are given in Chapter P-10 to specify the configuration of carbohydrates (see P-102.5.2.3), amino acids peptides (see P-103.1.3), and lipids (see P-107.4.3). Examples given in this Section are intended to illustrate the use of stereodescriptors for pseudoasymmetric stereogenic units and the treatment of nonstereogenic units.

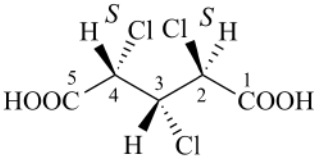
Examples:



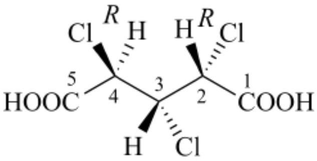
(2*R*,3*S*)-3-chloro-2-hydroxybutanoic acid (PIN)



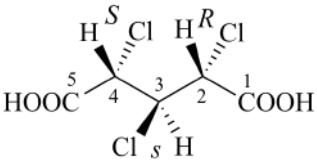
(2*S*,3*S*)-3-chloro-2-hydroxybutanoic acid (PIN)



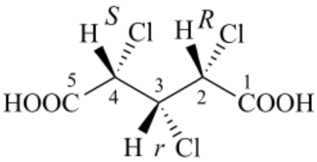
(2*S*,4*S*)-2,3,4-trichloropentanedioic acid (PIN)
(the nonstereogenic carbon atom 'C-3' is not identified by a stereodescriptor)



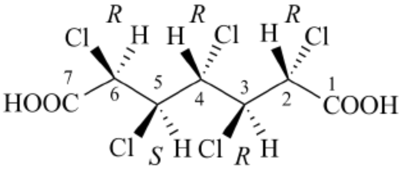
(2*R*,4*R*)-2,3,4-trichloropentanedioic acid (PIN)
(the nonstereogenic carbon atom 'C-3' is not identified by a stereodescriptor)



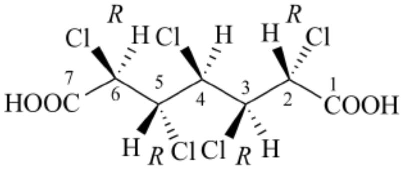
(2*R*,3*s*,4*S*)-2,3,4-trichloropentanedioic acid (PIN)
[chirality center '*R*' receives the lowest locant [see P-14.4 (j)];
application of Sequence Rule **5** generates the stereodescriptor '*s*' at 'C-3']



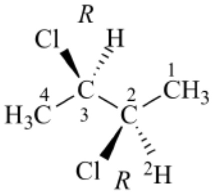
(2*R*,3*r*,4*S*)-2,3,4-trichloropentanedioic acid (PIN)
[chirality center '*R*' receives the lowest locant [see P-14.4 (j)];
application of Sequence Rule **5** generates stereodescriptor '*r*' at 'C-3'



(2*R*,3*R*,4*R*,5*S*,6*R*)-2,3,4,5,6-pentachloroheptanedioic acid (PIN)
[application of Sequence Rule **4** (‘*RR*’ > ‘*SR*’) generates stereodescriptor ‘*R*’ at C-4]



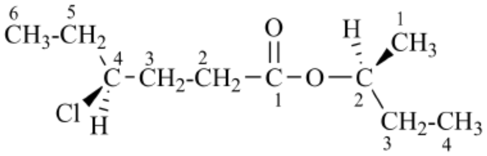
(2*R*,3*R*,5*R*,6*R*)-2,3,4,5,6-pentachloroheptanedioic acid (PIN)
(the carbon atom at C-4 is a nonstereogenic unit)



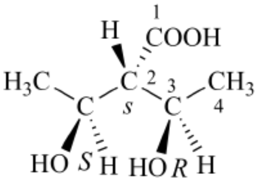
(2*R*,3*R*)-2,3-dichloro-(2-^{2}H)butane (PIN)

P-93.4.1.3 Stereodescriptors, if any, denoting the absolute configuration of a component cited as a prefix or in functional class names, are cited immediately before each respective component.

Examples:



(2*S*)-butan-2-yl (4*S*)-4-chlorohexanoate (PIN)



(2*s*,3*R*)-3-hydroxy-2-[(1*S*)-1-hydroxyethyl]butanoic acid (PIN)

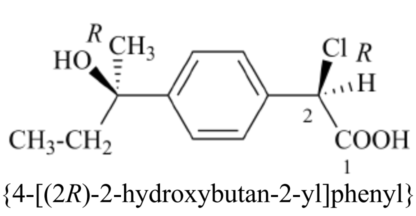
Explanation. Four steps are used in the construction of the stereospecific name:

Step 1: configurations ‘*R*’ and ‘*S*’ are assigned to the hydroxylated stereogenic centers;

Step 2: configuration ‘*s*’ is assigned to the pseudoasymetric stereogenic center;

Step 3: the principal chain has the maximum number of stereogenic centers having the ‘*R*’ configuration (see P-45.6.3);

Step 4: the name is constructed by citing the stereodescriptors at the front of the principal chain and of the substituent.



(2*R*)-2-chloro-2-{4-[(2*R*)-2-hydroxybutan-2-yl]phenyl}acetic acid (PIN)

P-93.4.2 Specification of configuration for double bonds

P-93.4.2.1 Specification of the configuration of double bonds
P-93.4.2.2 Allenes and cumulenes having an even number of double bonds
P-93.4.2.3 Cumulenes having an odd number of double bonds
P-93.4.2.4 Specification of configuration in unsaturated compounds containing multiple stereogenic units

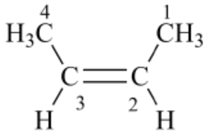
P-93.4.2.1 Specification of the configuration of double bonds

P-93.4.2.1.1 Stereodescriptors ‘*Z*’ and ‘*E*’, and ‘*cis*’ and ‘*trans*’

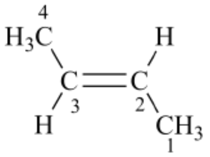
The stereodescriptors ‘*Z*’ and ‘*E*’ have been defined in section P-92.4; they are recommended to specify the configuration of double bonds as preferred stereodescriptors in preferred IUPAC names. Their use in nomenclature is described here. They have replaced the stereodescriptors ‘*cis*’ and ‘*trans*’ that are still recommended for general nomenclature and in the nomenclature of carotenoids.

The stereodescriptors ‘*cis*’ and ‘*trans*’ are used in general nomenclature only to describe double bonds having two hydrogen atoms, one on each carbon atom. Locants corresponding to those needed to describe a double bond are used before the stereodescriptors ‘*E*’ and ‘*Z*’, but not before ‘*cis*’ and ‘*trans*’. Locants are cited at the front of the stereodescriptor, followed by a hyphen; parentheses are used to nest the entire stereodescriptor.

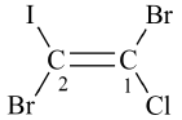
Examples:



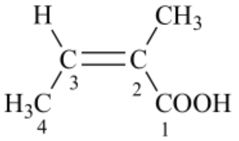
(2*Z*)-but-2-ene (PIN)
cis-but-2-ene



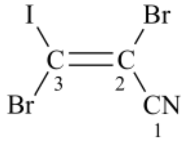
(2*E*)-but-2-ene (PIN)
trans-but-2-ene



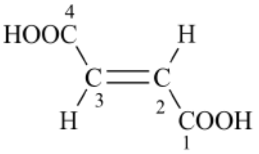
(1*Z*)-1,2-dibromo-1-chloro-2-iodoethene (PIN)



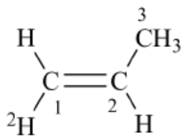
(2*Z*)-2-methylbut-2-enoic acid (PIN)



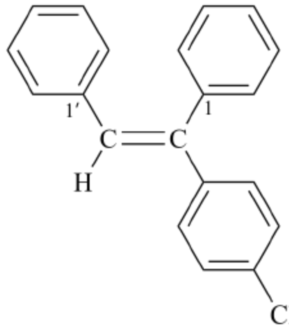
(2*Z*)-2,3-dibromo-3-iodoprop-2-enenitrile (PIN)
(2*Z*)-2,3-dibromo-3-iodoacrylonitrile



(2*E*)-but-2-enedioic acid (PIN;
fumaric acid (the configuration is implied in the retained name)



(1*E*)-(1-^{2}H$_{1}$)prop-1-ene (PIN)
trans-(1-^{2}H$_{1}$)prop-1-ene



1,1′-[(1*E*)-1-(4-chlorophenyl)ethene-1,2-diyl]dibenzene (PIN, see P-93.6)
4-chloro-1,1′-[(1*E*)-1-phenylethene-1,2-diyl]dibenzene

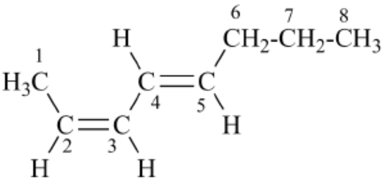
P-93.4.2.1.2 Compounds containing more than one double bond

The stereodescriptors '*E*' and '*Z*' related to the parent are cited, preceded by the appropriate locant if more than one double bond is present, before the complete name of the compound, or before the name of the appropriate component. Chain locants are used when double bonds are '*exo*' to the chain (see fifth example below). If more than one descriptor is used, the descriptors are cited in ascending order of their respective locants.

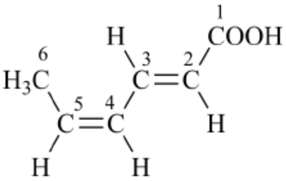
When alternative numberings of a chain or rings or ring systems are possible, that numbering is chosen which gives a '*cis*' attachment at the first point of difference. Attention must be given to the fact that a '*cis*' attachment is denoted by the stereodescriptor '*Z*'.

Stereodescriptors '*cis*' and '*trans*' may be used to describe double bonds having two hydrogen atoms, one on each carbon atom, but stereodescriptors '*E*' and '*Z*' are used in preferred IUPAC names. The stereodescriptors '*cis*' and '*trans*' are cited at the front of the name, preceded by the appropriate locant, if necessary, followed by a hyphen.

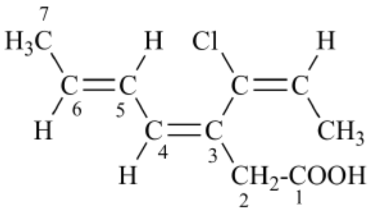
Examples:



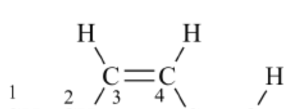
(2*Z*,4*E*)-octa-2,4-diene (PIN)
2-*cis*,4-*trans*-octa-2,4-diene



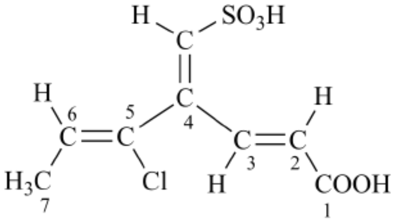
(2*E*,4*Z*)-hexa-2,4-dienoic acid (PIN)
2-*trans*,4-*cis*-hexa-2,4-dienoic acid



(3*Z*,5*E*)-3-[(1*E*)-1-chloroprop-1-en-1-yl]hepta-3,5-dienoic acid (PIN)



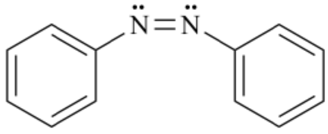
(3*Z*,5*E*)-octa-3,5-diene (PIN)
3-*cis*,5-*trans*-octa-3,5-diene
[the double bond with the *cis* configuration receives the lowest locants [see P-14.4 (j)]

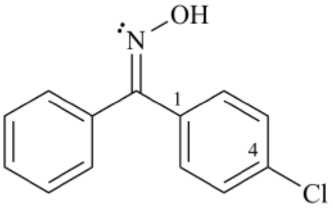

(2*E*,4*E*,5*Z*)-5-chloro-4-(sulfomethylidene)hepta-2,5-dienoic acid (PIN)

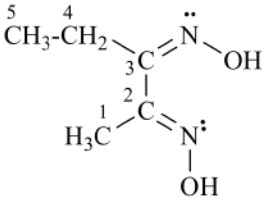
P-93.4.2.1.3 Descriptors '*E*' and '*Z*' to denote double bonds linked to heteroatoms

The stereodescriptors '*E*' and '*Z*' are also used to indicate the configuration of double bonds involving atoms other than carbon. A lone pair of electrons, when present, is considered to have the atomic number '0' (zero). The descriptors '*syn*' and '*anti*', and '*cis*' and '*trans*', are no longer recommended for these situations. No locant is required before the stereodescriptor when none is present in a name, but the stereodescriptor is placed in parentheses as indicated in P-91.3.

Examples:


(*Z*)-diphenyldiazene (PIN)
(not *cis*-diphenyldiazene)

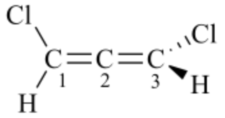

(*Z*)-*N*-hydroxy(4-chlorophenyl)(phenyl)methanimine (PIN)
(*Z*)-*N*-[(4-chlorophenyl)(phenyl)methylidene]hydroxylamine
(*Z*)-(4-chlorophenyl)(phenyl)methanone oxime

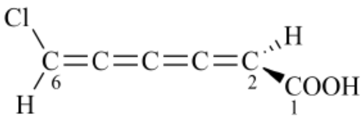

(2*E*,3*Z*)-N^2,N^3-dihydroxypentane-2,3-diimine (PIN)
(2*E*,3*Z*)-(pentane-2,3-diylidene)bis(hydroxylamine)
(2*E*,3*Z*)-pentane-2,3-dione dioxime

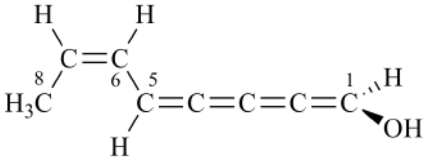
P-93.4.2.2 Allenes and cumulenes having an even number of double bonds

When appropriately substituted, allenes are chiral compounds having an axis of chirality. Chirality is thus described by the stereodescriptors 'R_a' and 'S_a' or '*M*' and '*P*', as described in P-92.1.2.1.2 and P-92.1.2.2.1, respectively. Stereodescriptors '*M*' and '*P*' are preferred to 'R_a' and 'S_a' in preferred IUPAC names. The stereodescriptor '*M*' or '*P*', describing the cumulene system, is preceded by a locant indicating the starting point of the cumulated double bond system having consecutive increasing locants differing by one unit. Compound locants are used only when locants are not consecutive as shown in P-93.5.2.3.

Examples:


(1*M*)-1,3-dichloropropa-1,2-diene (PIN)
(1R_a)-1,3-dichloropropa-1,2-diene


(2*P*)-6-chlorohexa-2,3,4,5-tetraenoic acid (PIN)
(2S_a)-6-chlorohexa-2,3,4,5-tetraenoic acid



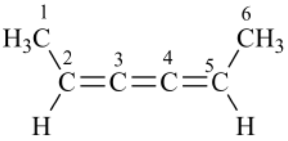
(1*P*,6*Z*)-octa-1,2,3,4,6-pentaen-1-ol (PIN)
(1*S*a,6*Z*)-octa-1,2,3,4,6-pentaen-1-ol

P-93.4.2.3 Cumulenes having an odd number of double bonds

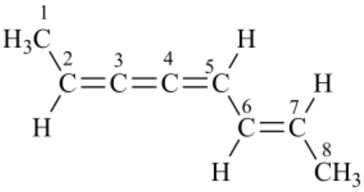
Cumulenes having an odd number of double bonds are planar molecules, like double bonds. The preferred stereodescriptors are '*E*' and '*Z*'. Stereodescriptors '*cis*' and '*trans*' may be used in general nomenclature.

The stereodescriptor '*E*' or '*Z*', describing the cumulene system, is preceded by a locant indicating the starting point of the cumulated double bond system having consecutive increasing locants differing by one unit. Compound locants are used only when locants are not consecutive as shown in P-93.5.2.3.

Examples:



(2*Z*)-hexa-2,3,4-triene (PIN)
cis-hexa-2,3,4-triene

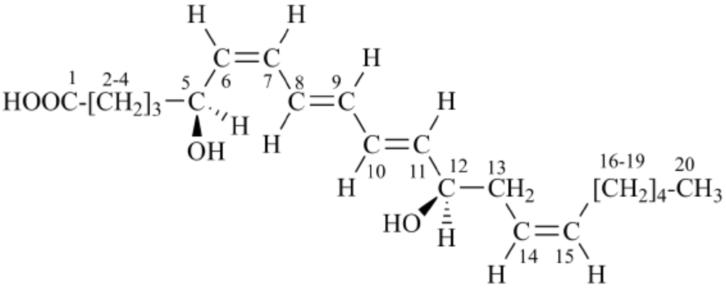


(2*E*,6*E*)-octa-2,3,4,6-tetraene (PIN)
2-*trans*,6-*trans*-octa-2,3,4,6-tetraene

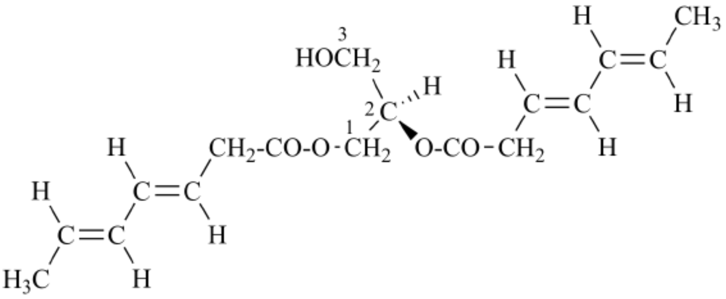
P-93.4.2.4 Specification of configuration in compounds with multiple stereogenic units

When chiral compounds contain multiple double bonds, >C=C<, stereodescriptors are assigned as described above. Stereodescriptors are cited at the front of the name or of any substituent group or appropriate portion of the name, in ascending order of the locants. For a discussion about the nomenclature of these unsaturated compounds, see P-92.4.2.

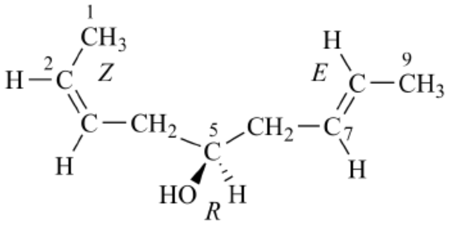
Examples:



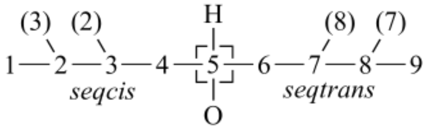
(5*S*,6*Z*,8*E*,10*E*,12*R*,14*Z*)-5,12-dihydroxyicosa-6,8,10,14-tetraenoic acid (PIN)
6-*cis*,8-*trans*,10-*trans*,14-*cis*-(5*S*,12*R*)-5,12-dihydroxyicosa-6,8,10,14-tetraenoic acid



(2*R*)-3-hydroxypropane-1,2-diyl di[(3*E*,5*E*)-hepta-3,5-dienoate] (PIN)
(2*R*)-3-hydroxypropane-1,2-diyl di(3-*trans*,5-*trans*-hepta-3,5-dienoate)



(2*Z*,5*R*,7*E*)-nona-2,7-dien-5-ol (PIN)



simplified digraph

P-93.5 CONFIGURATION SPECIFICATION OF CYCLIC ORGANIC COMPOUNDS

- P-93.5.0 Introduction
- P-93.5.1 Monocyclic compounds
- P-93.5.2 von Baeyer compounds
- P-93.5.3 Spiro compounds
- P-93.5.4 Fused and bridged fused compounds
- P-93.5.5 Cyclophanes
- P-93.5.6 Fullerenes
- P-93.5.7 Ring assemblies

P-93.5.0 Introduction

The application of CIP stereodescriptors to monocyclic compounds is discussed in this section. Stereodescriptors used before the CIP system was established are still recommended for general nomenclature and are mandatory in the field of Natural Products as indicated in Chapter P-10.

The following non-CIP stereodescriptors are used in general IUPAC substitutive nomenclature: '*cis*', '*trans*' (see P-93.5.1.2); '*r*', '*c*', '*t*' (see P-93.5.1.3); '*endo*', '*exo*', '*syn*', '*anti*' (see P-93.5.2.2.1).

P-93.5.1 Monocyclic compounds

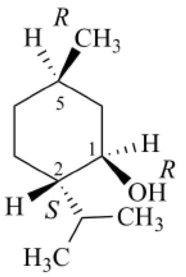
- P-93.5.1.1 Specification of stereogenic centers: stereodescriptors '*R*', '*S*', '*r*', and '*s*'
- P-93.5.1.2 Relative configuration: stereodescriptors '*cis*' and '*trans*'
- P-93.5.1.3 Relative configuration: stereodescriptors '*r*', '*c*', and '*t*'
- P-93.5.1.4 Unsaturated alicyclic compounds

P-93.5.1.1 Specification of stereogenic centers: stereodescriptors '*R*', '*S*', '*r*', and '*s*'

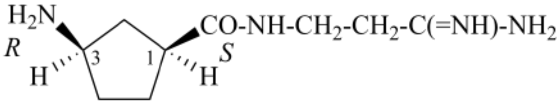
P-93.5.1.1.1 Absolute configuration

In substituted monocyclic compounds the absolute configuration is specified in preferred IUPAC names by the CIP stereodescriptors such as '*R*', '*S*', '*r*', and '*s*'.

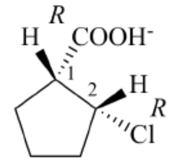
Examples:



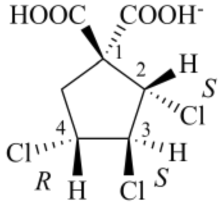
(1*R*,2*S*,5*R*)-5-methyl-2-(propan-2-yl)cyclohexan-1-ol (PIN)



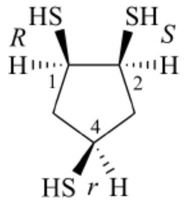
(1*S*,3*R*)-3-amino-*N*-(3-amino-3-iminopropyl)cyclopentane-1-carboxamide (PIN)


R
H
COOH-
1
2
H
R
Cl

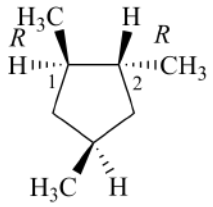
(1*R*,2*R*)-2-chlorocyclopentane-1-carboxylic acid (PIN)


HOOC
COOH-
1
2
H
S
Cl
4
3
Cl
H
R
H
Cl
S

(2*S*,3*S*,4*R*)-2,3,4-trichlorocyclopentane-1,1-dicarboxylic acid (PIN)


HS
SH
R
S
H
H
1
2
4
HS
r
H

(1*R*,2*S*,4*r*)-cyclopentane-1,2,4-trithiol (PIN)


H3C
H
R
R
H
CH3
1
2
H3C
H

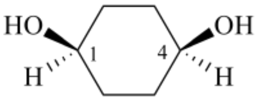
(1*R*,2*R*)-1,2,4-trimethylcyclopentane (PIN)
(no stereodescriptor is assigned to C-4; it is a nonstereogenic center)

P-93.5.1.1.2 Achiral cyclic compounds

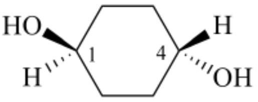
The configuration of achiral cyclic molecules is also specified by CIP stereodescriptors in preferred IUPAC names.

(a) The configuration at pseudoasymmetric centers, for example, at ‘C-1’ and ‘C-4’ of 1,4-disubstituted cyclohexanes, is specified by the methodology discussed in Example 2 in P-92.6.

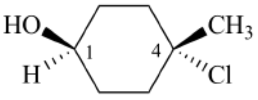
Examples:



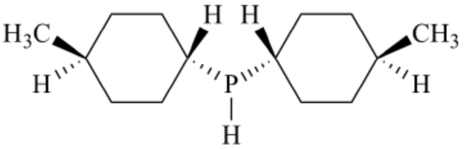
(1*s*,4*s*)-cyclohexane-1,4-diol (PIN)
cis-cyclohexane-1,4-diol



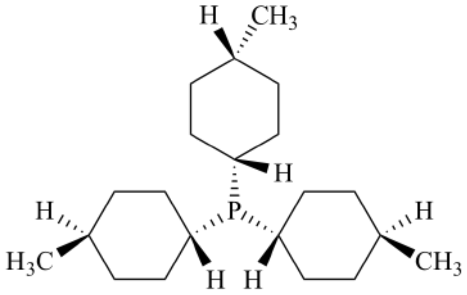
(1*r*,4*r*)-cyclohexane-1,4-diol (PIN)
trans-cyclohexane-1,4-diol


HO
CH3
1
4
H
Cl

(1*r*,4*r*)-4-chloro-4-methylcyclohexan-1-ol (PIN)
trans-4-chloro-4-methylcyclohexan-1-ol

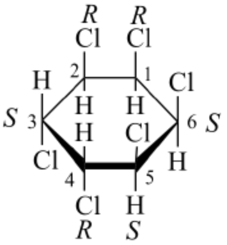

H3C
H H
CH3
H
P
H
H

bis[(1*r*,4*r*)-4-methylcyclohexyl]phosphane (PIN)
bis(*trans*-4-methylcyclohexyl)phosphane

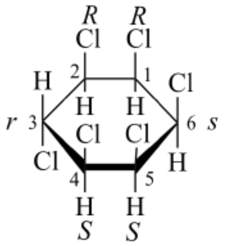

H
CH3
H
P
H
H3C
H
H
H
CH3

bis[(1*r*,4*r*)-4-methylcyclohexyl][(1*s*,4*s*)-4-methylcyclohexyl]phosphane (PIN)
(*cis*-4-methylcyclohexyl)bis(*trans*-4-methylcyclohexyl)phosphane

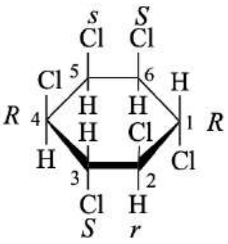
(b) The achiral isomers of 1,2,3,4,5,6-hexasubstituted cyclohexane by identical substituents are described below. By the method described in P-92.5, for the chiral isomer, Sequence Rule **4** is applied exhaustively; then, Sequence Rule **5** (see P-92.6) is used to name pseudoasymmetric stereogenic centers. Stereodescriptor sets of CIP stereodescriptors are described for each diastereoisomer, numbered 1 through 7; they are to be inserted at the front of the substitutive name, as shown here for the first enantiomer in the series shown below: (1*R*,2*R*,3*S*,4*R*,5*S*,6*S*)-1,2,3,4,5,6-hexachlorocyclohexane (see P-93.5.1.3.2 for the preferred IUPAC name, 1,2,3,4,5,6-hexachlorocyclohexane). The numbering for these examples is decided by application of criterion P-14.4 (j).


R R
Cl Cl
H 2 1 Cl
H H
S 3 6 S
H Cl
Cl 4 5 H
Cl H
R S

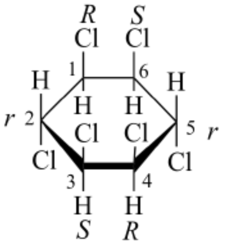
1 (1*R*,2*R*,3*S*,4*R*,5*S*,6*S*)


R R
Cl Cl
H 2 1 Cl
H H
r 3 6 s
Cl Cl
Cl 4 5 H
H H
S S

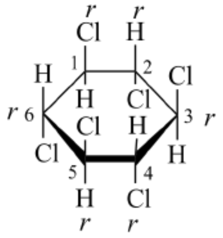
2 (1*R*,2*R*,3*r*,4*S*,5*S*,6*s*)


s S
Cl Cl
Cl 5 6 H
H H
R 4 1 R
H Cl
H 3 2 Cl
Cl H
S r

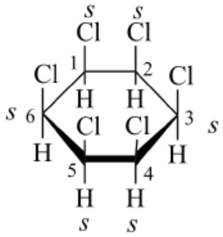
3 (1*R*,2*S*,3*r*,4*R*,5*S*,6*s*)
Note *R* > *r* > *S* > *s* [see P-14.4 (j)]


R S
Cl Cl
H 1 6 H
H H
r 2 5 r
Cl Cl
Cl 3 4 Cl
H H
S R

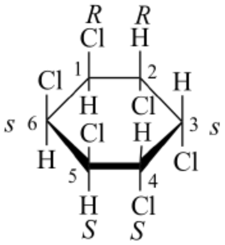
4 (1*R*,2*r*,3*S*,4*R*,5*r*,6*S*)
Note *R* > *r* > *S* > *s* [see P-14.4 (j)]



5 (1*r*,2*r*,3*r*,4*r*,5*r*,6*r*)



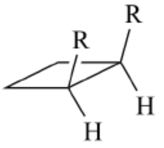
6 (1*s*,2*s*,3*s*,4*s*,5*s*,6*s*)



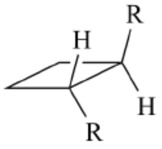
7 (1*R*,2*R*,3*s*,4*S*,5*S*,6*s*)

P-93.5.1.2 Relative configuration: the stereodescriptors '*cis*' and '*trans*'

The stereodescriptors '*cis*' and '*trans*' are used to show the relationship between two ligands (atoms or groups) attached to separate atoms that are contained in a ring or a ring system. The two ligands are said to be located '*cis*' to each other if they lie on the same side of a plane. If they are on opposite sides, their relative position is described as '*trans*'. The appropriate reference plane of a ring or ring system (the ring being in a conformation, real or assumed, without reentrant angles at the two substituted atoms) is the mean plane of the ring(s). The stereodescriptors denote relative configuration; the absolute configuration must be described by CIP stereodescriptors such as '*R*' and '*S*'.

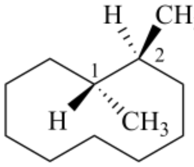


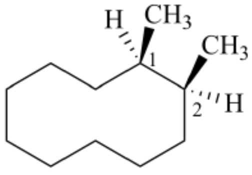
cis



trans

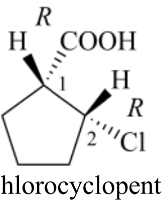
The structures below look like '*cis/trans*-isomers', but are actually different conformations of the same '*cis*' stereoisomer. In the conformation on the left hand side, the stereogenic center at 'C-1' is located on a reentrant angle.





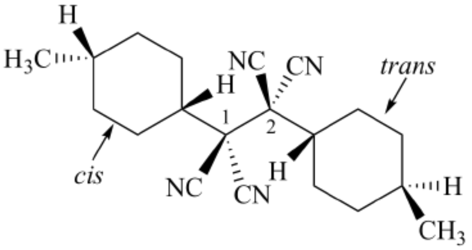
When one ligand and one hydrogen atom are attached at each of two positions of a monocycle, the steric relation (the relative configuration) of the two ligands is expressed as '*cis*' or '*trans*', followed by a hyphen and placed before the name of the compound. No locants are required before the stereodescriptors. In names, '*cis*' arrangements of ligands are cited before '*trans*' isomers, when a choice is possible. To describe the relative configuration the stereodescriptors '*R*' and '*S*' preceded by the term '*rel*' are preferred to '*R**'and '*S**', and also to '*cis*' and '*trans*' (see P-93.1.2).

Examples:

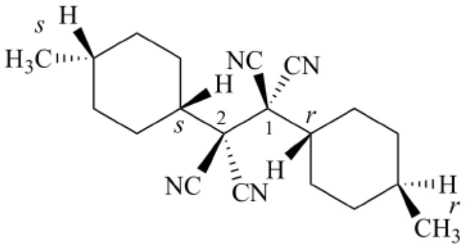


or enantiomer

cis-2-chlorocyclopentane-1-carboxylic acid
rel-(1*R*,2*R*)-2-chlorocyclopentane-1-carboxylic acid (PIN)
(1*R**,2*R**)-2-chlorocyclopentane-1-carboxylic acid
[not *rel*-(1*S*,2*S*)-2-chlorocyclopentane-1-carboxylic acid]
[not (1*S**,2*S**)-2-chlorocyclopentane-1-carboxylic acid]



I



II

(**I**) 1-(*cis*-4-methylcyclohexyl)-2-(*trans*-4-methylcyclohexyl)ethane-1,1,2,2-tetracarbonitrile
(**II**) 1-[(1*r*,4*r*)-4-methylcyclohexyl]-2-[(1*s*,4*s*)-4-methylcyclohexyl]ethane-1,1,2,2-tetracarbonitrile (PIN; the use of CIP stereodescriptors generates the preferred IUPAC name)

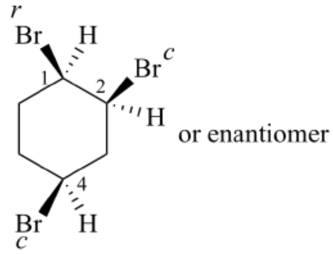
Explanation: In structure **I**, the locant '1' is assigned to the non-CIP stereodescriptor '*cis*'; and in structure **II** to the CIP stereodescriptor '*r*'. In names, the stereodescriptor '*cis*' is cited before '*trans*' and '*r*' before '*s*'.

P-93.5.1.3 Relative configuration; the stereodescriptors '*r*', '*c*', and '*t*'

P-93.5.1.3.1 When one substituent and one hydrogen atom are attached to each of more than two positions of a monocycle, the steric relations of the ligands are expressed by adding '*r*' (the reference ligand) after the locant of the lowest numbered of these ligands, and '*c*' for '*cis*' and '*t*' for '*trans*' (as required) after the locant of another ligand, thus expressing the relationship to the reference ligand. The relative configuration is expressed by these stereodescriptors. Furthermore, racemates may also be denoted by this method. For preferred IUPAC names, the preferred stereodescriptors are those used in the CIP priority system described in P-91 and P-92, with stereodescriptors such as '*R*' and '*S*' to describe absolute configuration and the prefixes '*rel*' to express relative configuration and '*rac*' for racemates, as described in P-93.1.3.

The notation consisting of adding '*r*' (for reference substituent) after the locant of the lowest numbered of these substituents and '*c*' (for *cis*) and '*t*' (for *trans*) (as appropriate) and the locant for another substituent, as used in the 1993 Guide to IUPAC Nomenclature of Organic Compounds (ref. 2), is no longer recommended.

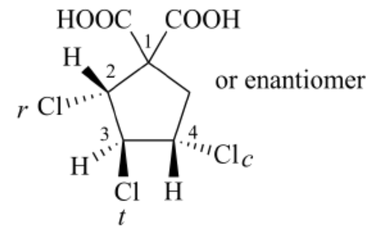
Example 1:



or enantiomer

1*r*,2*c*,4*c*-tribromocyclohexane
rel-(1*R*,2*S*,4*S*)-1,2,4-tribromocyclohexane (PIN)

Example 2:

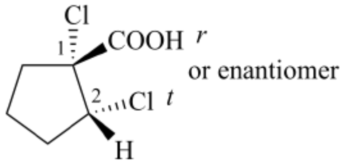


or enantiomer

2*r*,3*t*,4*c*-trichlorocyclopentane-1,1-dicarboxylic acid
rel-(2*R*,3*R*,4*S*)-2,3,4-trichlorocyclopentane-1,1-dicarboxylic acid (PIN)
(2*R**,3*R**,4*S**)-2,3,4-trichlorocyclopentane-1,1-dicarboxylic acid
[not *rel*-(2*S*,3*S*,4*R*)-2,3,4-trichlorocyclopentane-1,1-dicarboxylic acid; the lowest locant must be specified by a '*R*' stereodescriptor]
[not (2*S**,3*S**,4*R**)-2,3,4-trichlorocyclopentane-1,1-dicarboxylic acid; the lowest locant must be specified by a '*R**' stereodescriptor]

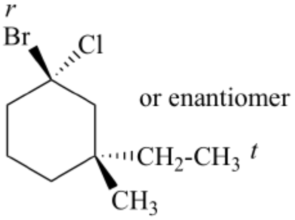
P-93.5.1.3.2 When two different ligands are attached at the same position of a monocycle, then the lowest-numbered ligand named as a suffix is chosen as reference ligand. If none of the ligands is named as a suffix, then one of the ligands having the lowest locant and higher ranking in the Sequence Rule is chosen as a reference ligand. The relationship of the Sequence-Rule-higher ranking at geminally substituted positions, relative to the reference group, is cited as '*c*' or '*t*', as required.

Example 1:



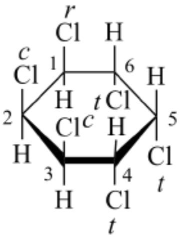
1,2*t*-dichlorocyclopentane-1*r*-carboxylic acid
rel-(1*R*,2*R*)-1,2-dichlorocyclopentane-1-carboxylic acid (PIN)

Example 2:



1*r*-bromo-1-chloro-3*t*-ethyl-3-methylcyclohexane
rel-(1*R*,3*R*)-1-bromo-1-chloro-3-ethyl-3-methylcyclohexane (PIN)
(1*R**,3*R**)-1-bromo-1-chloro-3-ethyl-3-methylcyclohexane

Example 3:



(1*R*,2*R*,3*s*,4*S*,5*S*,6*s*)-1,2,3,4,5,6-hexachlorocyclohexane (PIN)
1*r*,2*c*,3*c*,4*t*,5*t*,6*t*-hexachlorocyclohexane

Explanation: In this compound, different numberings are necessary in accordance with the precedence of '*R*' ligands and '*cis*' arrangements for lowest locants [this compound is example 7 discussed in P-93.5.1.1.2 (b); other isomers are described in P-92.5.2.2 and P-93.5.1.1.2 (b).]

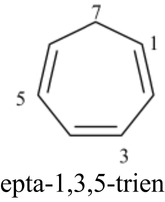
P-93.5.1.4 Unsaturated alicyclic compounds

P-93.5.1.4.1 Specification of cyclic double bonds
P-93.5.1.4.2 Specification of *exo*-cyclic double bonds

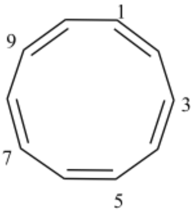
P-93.5.1.4.1 Specification of cyclic double bonds

In three- to seven-membered monocycles, cyclic double bonds have a '*cis*' configuration; the stereodescriptor, '*Z*' or '*cis*', denoting the configuration of the cyclic double bonds (double bonds that are included in the ring) is permanently omitted. From eight-membered monocycles members onward, cyclic double bonds can be either '*cis*' or '*trans*'; the stereodescriptors '*Z*' and '*E*', must be used in preferred IUPAC names, to specify such arrangements; the stereodescriptors '*cis*' and '*trans*' may be used in general nomenclature.

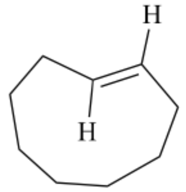
Examples:



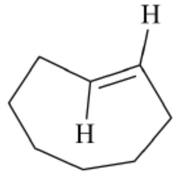
cyclohepta-1,3,5-triene (PIN)



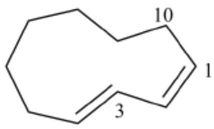
(1*Z*,3*Z*,5*Z*,7*Z*,9*Z*)-cyclodeca-1,3,5,7,9-pentaene (PIN)



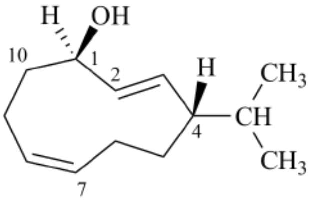
(*E*)-cyclononene (PIN)



(*E*)-cyclooctene (PIN)



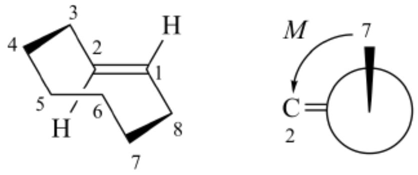
(1*Z*,3*E*)-cyclodeca-1,3-diene (PIN)
1-*cis*,3-*trans*-cyclodeca-1,3-diene
[lowest locants are assigned to the '*Z*' double bond; see P-14.4 (j)]



(1*R*,2*E*,4*S*,7*Z*)-4-(propan-2-yl)cyclodeca-2,7-dien-1-ol (PIN)
2-*trans*,7-*cis*-(1*R*,4*S*)-4-(propan-2-yl)cyclodeca-2,7-dien-1-ol

The stereodescriptors '*M*', '*P*', 'R_p', or 'S_p' are used to denote the configuration of '*E*' chiral isomers of cycloalkenes. The stereodescriptors '*M*' and '*P*' are used in preferred IUPAC names.

Example:



(1*E*,1*M*)-cyclooct-1-ene (PIN)
(*E*,*M*)-cyclooctene
(*E*,S_p)-cyclooctene

P-93.5.1.4.2 Specification of *exo*-cyclic double bonds

P-93.5.1.4.2.1 Specification by stereodescriptors '*E*' and '*Z*'

The stereodescriptors '*E*' and '*Z*' are used to specify the configuration of an *exo*-cyclic double bond.

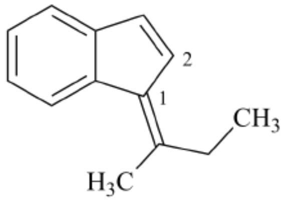
(1) When one double bond is present, two methods are used to construct the names

(a) the double bond is considered as an integral part of the parent structure; the stereodescriptor is placed at the front of the substitutive name, preceded by the locant indicating its point of attachment to the parent structure;

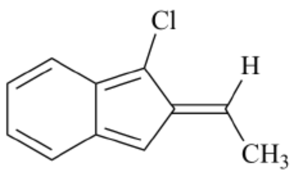
(b) the double bond is considered as part of the substituent group of the 'ylidene' type. The stereodescriptor is cited at the front of the name of the substituent group; the name of the corresponding prefix is then placed in enclosing marks.

Method (a) generates preferred IUPAC names.

Examples:



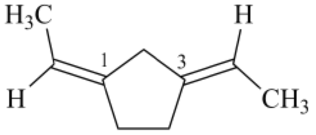
(1*E*)-1-(butan-2-ylidene)-1*H*-indene (PIN)
[(2*E*)-butan-2-ylidene]-1*H*-indene



(2*E*)-1-chloro-2-ethylidene-2*H*-indene (PIN)
1-chloro-2-[(*E*)-ethylidene]-2*H*-indene

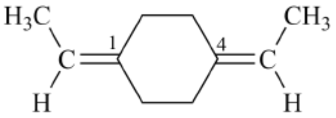
(2) When two double bonds are attached to the same ring, the two methods described in (1) are applied. Each double bond is specified by method (a) in preferred IUPAC names. A third method is also used in general nomenclature, in which the ring is considered as a formal double bond and the entire system specified as a cumulene with an odd number of double bonds (see P-93.4.2.3). This method is only valid with a 2*n*-membered monocyclic ring substituted in opposite positions. Otherwise method (a) is used.

Example 1:


H3C
H
1
3
H
CH3

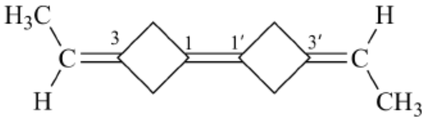
(1*Z*,3*E*)-1,3-diethylidenecyclopentane (PIN)
1-[(*Z*)-ethylidene]-3-[(*E*)-ethylidene]cyclopentane

Example 2:


H3C
CH3
C
1
4
C
H
H

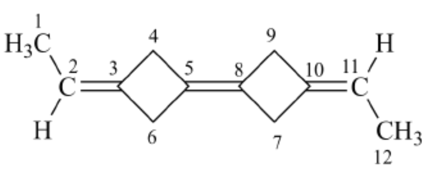
(1*Z*,4*Z*)-1,4-diethylidenecyclohexane (PIN)
(see Example 1 in P-92.4.2.2 for specifying a ‘*Z*’ configuration at ‘C-1’ and ‘C-4’)
cis-1,4-diethylidenecyclohexane
1,4-di[(*Z*)-ethylidene]cyclohexane

Example 3:

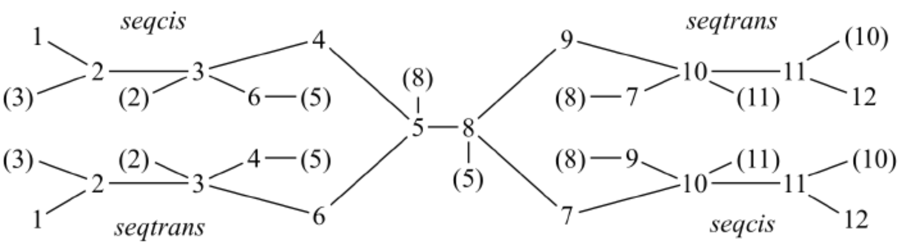

H3C
C
H
3
1
1′
3′
H
C
CH3

[1(1′)*E*,3*E*,3′*E*]-3,3′-diethylidene-1,1′-bi(cyclobutylidene) (PIN)
trans-3,3′-diethylidene-1,1′-bi(cyclobutylidene)
3,3′-di[(*E*)-ethylidene]-1,1′-bi(cyclobutylidene)

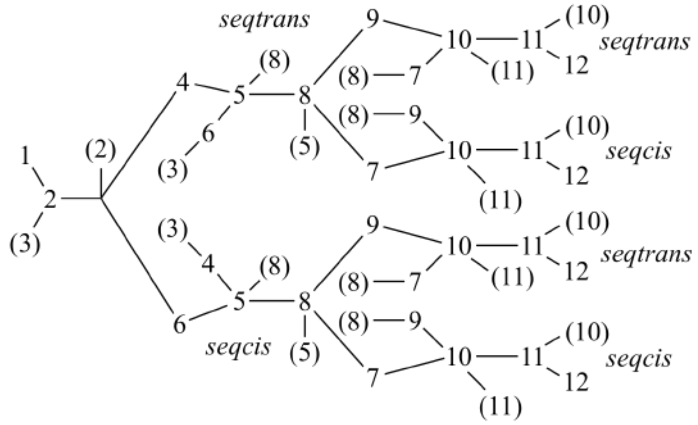
Explanation:


1
H3C
2
C
H
3
4
6
5
8
9
7
10
11
H
C
CH3
12

arbitrarily renumbered structure in order to establish the required digraphs:


seqcis
1
2
(3)
(2)
3
4
6
(5)
(8)
5
8
(5)
9
seqtrans
10
11
(10)
(8)
7
(11)
12
(3)
2
1
(2)
3
4
(5)
6
seqtrans
(8)
9
10
(11)
11
(10)
7
seqcis
12

simplified digraph for 5 and 8 in the renumbered structure



simplified digraph for 2 and 3 in the renumbered structure

P-93.5.1.4.2.2 Specification of *exo*-cyclic double bonds by stereodescriptors other than '*E*' and '*Z*'.

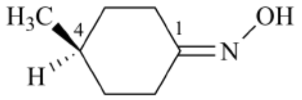
Compounds composed of a substituted ring and an *exo*-cyclic double bond can be considered as an allene system and named in two ways:

(1) by identifying and specifying individual stereogenic units

(2) by considering the entire molecule as a unique system and naming as such

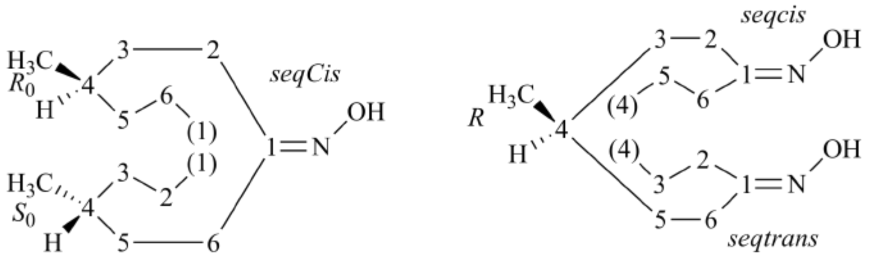
IUPAC names are based on method (1).

Example 1:



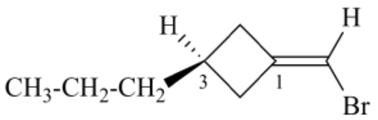
(1*seqCis*,4*R*)-*N*-hydroxy-4-methylcyclohexan-1-imine (PIN)
[(1*seqCis*,4*R*)-4-methylcyclohexylidene]hydroxylamine
[for '*seqCis*' see P-92.1.1 (f)]
(*M*)-(4-methylcyclohexylidene)hydroxylamine
(R_{a})-4-methylcyclohexanone oxime

Explanation: The following digraphs are used for specifying the configurations 'C-1' and 'C-4':



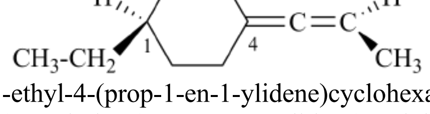
C-1 simplified digraphs C-4

Example 2:



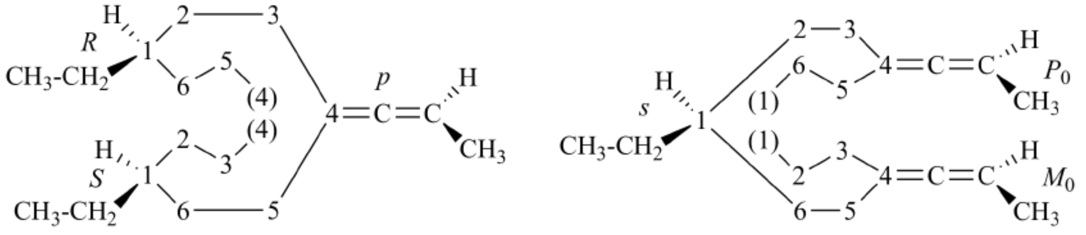
(1*seqCis*,3*S*)-1-(bromomethylidene)-3-propylcyclobutane (PIN)
(*P*)-1-(bromomethylidene)-3-propylcyclobutane
(S_{a})-1-(bromomethylidene)-3-propylcyclobutane

Example 3:



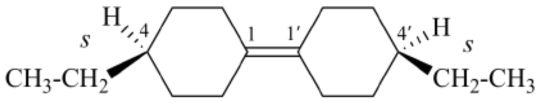
(1*s*,4*p*)-1-ethyl-4-(prop-1-en-1-ylidene)cyclohexane (PIN)
(1*s*,4s_{a})-1-ethyl-4-(prop-1-en-1-ylidene)cyclohexane

Explanation: The following digraphs are used for specifying the configurations 'C-1' and 'C-4':



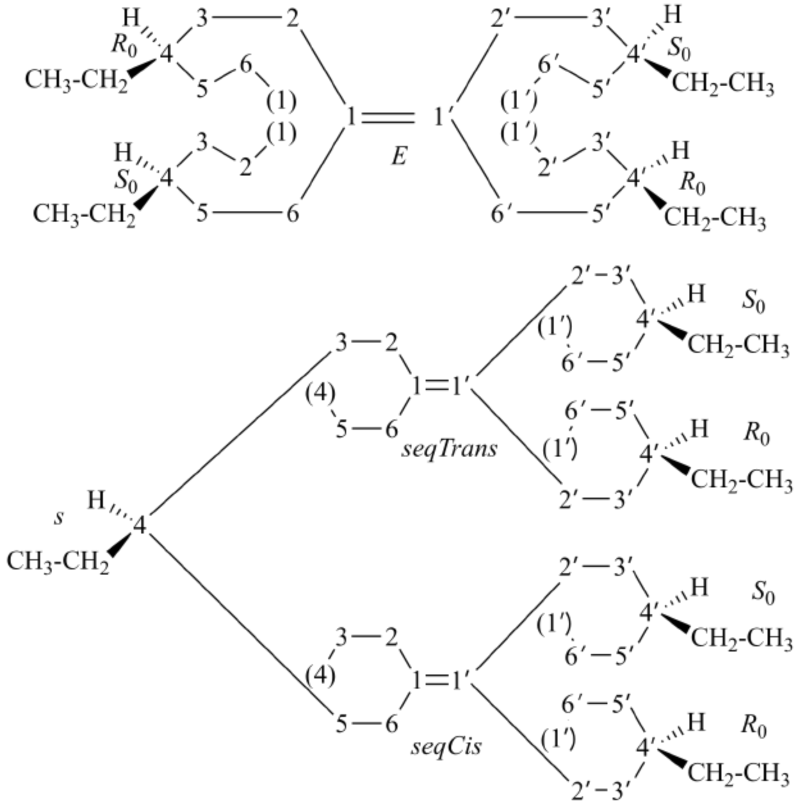
C-4 simplified digraphs C-1

Example 4:



[1(1′)*E*,4*s*,4′*s*]-4,4′-diethyl-1,1′-bi(cyclohexylidene) (PIN)
(4*s*,4′*s*)-4,4′-diethyl-1,1′-bi(cyclohexylidene)
cis-4,4′-diethyl-1,1′-bi(cyclohexylidene)

Explanation: The following digraphs are used in the specification of the configuration at the stereogenic double bond and the stereogenic center ‘C-4’ (shown):



simplified digraphs

Explanation: The configuration of the double bond ‘C-1=C-1′’ is determined as follows. The auxiliary stereodescriptors on each side of the double bond are ‘R_0’ and ‘S_0’; priority being given to ‘R_0’ over ‘S_0’, the ligands ‘2’ and ‘6′’ permit an ‘*E*’ configuration to be assigned. The configuration at ‘C-4’ is determined as follows. In the digraph, the configurations ‘R_0’ and ‘S_0’ permit, in each branch the determination of the configuration of the auxiliary stereodescriptor ‘*seqCis*’ and ‘*seqTrans*’ for the double bonds ‘C-1=C-1′’; priority being assigned to ‘*seqCis*’ according to Sequence Rule **5**, the ligand ‘C-5’ has priority over ligand ‘C-3’, thus permitting the configuration ‘*s*’ to be assigned according to Sequence Rule **5**.

Note: While there is a *cis* arrangement of substituents, CIP descriptors include *E*, which cannot be used alone, to describe the configuration of the structure.

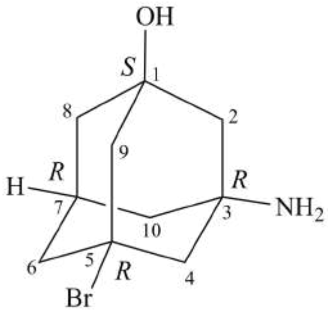
P-93.5.2 von Baeyer compounds

P-93.5.2.1 Specification of stereogenic centers by CIP stereodescriptors
P-93.5.2.2 Relative configuration
P-93.5.2.3 Specification of double bonds

P-93.5.2.1 Specification of stereogenic centers by CIP stereodescriptors

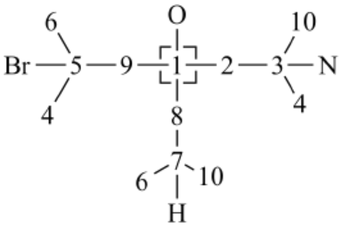
The absolute configuration with a unique numbering determined by the structure is specified by CIP stereodescriptor such as‘*R*’, ‘*s*’, etc.

Examples:



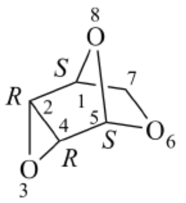
OH
S
1
8
2
9
H
R
R
7
3
NH$_2$
10
6
5
R
4
Br

(1*S*,3*R*,5*R*,7*R*)-3-amino-5-bromoadamantan-1-ol (PIN)
(1*S*,3*R*,5*R*,7*R*)-3-amino-5-bromotricyclo[3.3.1.1^{3,7}]decan-1-ol



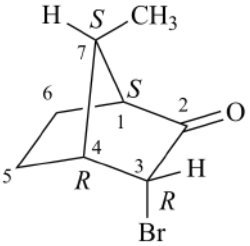
6
O
10
Br
5
9
1
2
3
N
4
8
4
7
6
10
H

simplified digraph



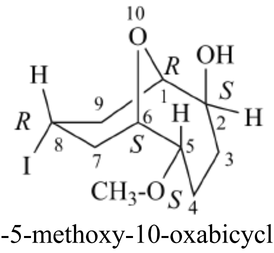
8
O
S
7
R
2
1
4
5
O$_6$
S
O
R
3

(1*S*,2*R*,4*R*,5*S*)-3,6,8-trioxatricyclo[3.2.1.0^{2,4}]octane (PIN)



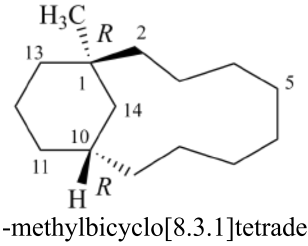
H
S
CH$_3$
7
6
S
2
O
1
4
5
3
H
R
R
Br

(1*S*,3*R*,4*R*,7*S*)-3-bromo-7-methylbicyclo[2.2.1]heptan-2-one (PIN)



10
O
R
OH
H
S
9
1
R
6
H
2
H
8
S
5
3
I
7
CH$_3$-O
S
4

(1*R*,2*S*,5*S*,6*S*,8*R*)-8-iodo-5-methoxy-10-oxabicyclo[4.3.1]decan-2-ol (PIN)



H$_3$C
R
2
13
1
5
14
10
11
R
H

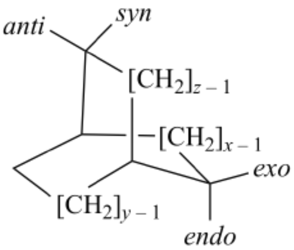
(1*R*,10*R*)-1-methylbicyclo[8.3.1]tetradecane (PIN)

P-93.5.2.2 Relative configuration

Relative configuration and racemates are specified by using the stereodescriptors ‘*R*’ and ‘*S*’ and prefixes ‘*rel*’ and ‘*rac*’ as described in P-93.1.2 and P-93.1.3.

P-93.5.2.2.1 The stereodescriptors ‘*endo*’, ‘*exo*’, ‘*syn*’, and ‘*anti*’

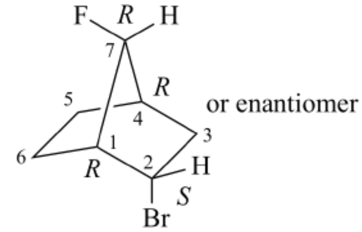
These stereodescriptors are used to indicate the relative orientation of groups attached to nonbridgehead atoms in bicyclo[x.y.z]alkanes, where ‘$x \geq y > z > 0$’, and with the additional provision that the two bridges ‘$x + y$’ must be smaller than ‘7’. In fact, these stereodescriptors are used to describe the relative configuration of bi- and tricyclic systems such as bicyclo[2.2.1]heptanes, bicyclo[3.2.1]octane, and bicyclo[3.3.1]nonane.



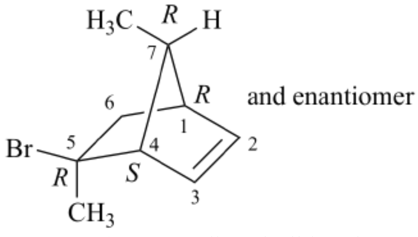
If the substituent is orientated toward the highest numbered bridge (‘*Z*’ bridge, e.g. ‘C-7’ in example below) it is given the description ‘*exo*’; if it is orientated away from the highest numbered bridge it is given the description ‘*endo*’. If the substituent is attached to the highest numbered bridge and is orientated toward the lowest numbered bridge (‘x’ bridge, e.g. ‘C-2’ in example below) it is given the description ‘*syn*’; if the substituent is orientated away from the lowest numbered bridge it is given the description ‘*anti*’. In names, the stereodescriptors are cited between the locant and the substituent, with connecting hyphens.

The stereodescriptors ‘*endo*’, ‘*exo*’, ‘*syn*’, and ‘*anti*’ describe relative configuration only; they do not permit to distinguish between a single enantiomer (first example below) and a racemate (second example below); the phrase ‘and/or enantiomer’ is used to denote these two possibilities. The absolute configuration must be described by CIP stereodescriptors such as ‘*R*’ and ‘*S*’; these stereodescriptors, accompanied by the prefixes ‘*rel*’ and ‘*rac*’, permit a full description of any given compound.

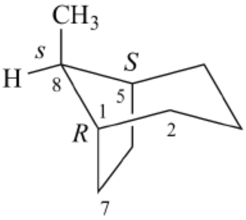
Examples:



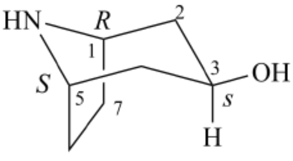
2-*endo*-bromo-7-*anti*-fluorobicyclo[2.2.1]heptane
rel-(1*R*,2*S*,4*R*,7*R*)-2-bromo-7-fluorobicyclo[2.2.1]heptane (PIN)



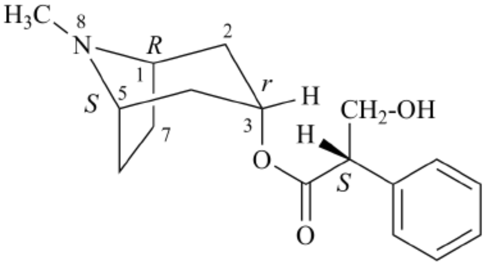
(±)-5-*exo*-bromo-5-*endo*,7-*anti*-dimethylbicyclo[2.2.1]hept-2-ene
rac-(1*R*,4*S*,5*S*,7*R*)-5-bromo-5,7-dimethylbicyclo[2.2.1]hept-2-ene (PIN)



8-*syn*-methylbicyclo[3.2.1]octane
(1*R*,5*S*,8*s*)-8-methylbicyclo[3.2.1]octane (PIN)



(1*R*,3*s*,5*S*)-8-azabicyclo[3.2.1]octan-3-ol
(3*s*)-8-nortropan-3-ol
8-azabicyclo[3.2.1]octan-3-*exo*-ol

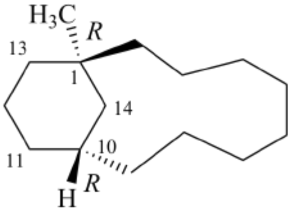


(1*R*,3*r*,5*S*)-8-methyl-8-azabicyclo[3.2.1]octan-3-yl (2*S*)-3-hydroxy-2-phenylpropanoate
8-methyl-8-azabicyclo[3.2.1]octan-3-*endo*-yl (2*S*)-3-hydroxy-2-phenylpropanoate
tropan-3α-yl (2*S*)-3-hydroxy-2-phenylpropanoate (see P-101.7.3)

P-93.5.2.2.2 Stereodescriptors '*cis*' and '*trans*'

Stereodescriptors '*cis*' and '*trans*' can be used in general nomenclature only to specify the '*cis*' or '*trans*' arrangement of ligands on bridgeheads. CIP stereodescriptors, preceded by the prefix '*rel*', must be used in association with preferred IUPAC names.

Example:



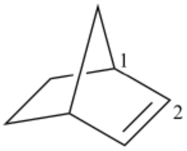
or enantiomer

rel-(1*R*,10*R*)-1-methylbicyclo[8.3.1]tetradecane (PIN)
(1*R**,10*R**)-1-methylbicyclo[8.3.1]tetradecane
1-methyl-*trans*-bicyclo[8.3.1]tetradecane

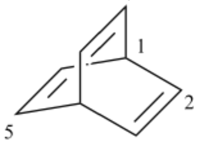
P-93.5.2.3 Specification of double bonds

As described for cycloalkenes (see P-93.5.1.4.1), in unsaturated bicyclo[3.3.3]undecane and smaller systems, it is not necessary to identify the configuration of double bonds as '*Z*'. All double bonds in larger systems need to be specified as '*Z*' or '*E*'.

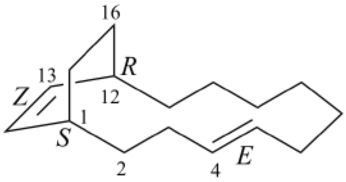
Examples:



bicyclo[2.2.1]hept-2-ene (PIN)

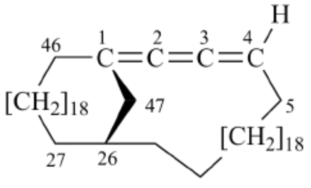


bicyclo[2.2.2]octa-2,5,7-triene (PIN)

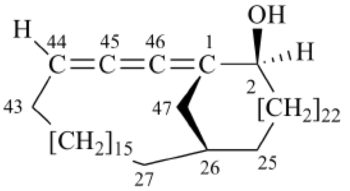


(1*S*,4*E*,12*R*,13*Z*)-bicyclo[10.2.2]hexadeca-4,13-diene (PIN)
(1*S*,4*E*,12*R*)-bicyclo[10.2.2]hexadeca-4,13-diene

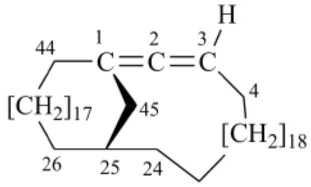
Cumulene systems included in cyclic systems are treated as discussed in P-93.4.2.2 and P-93.4.2.3 and numbered according to the numbering of the cyclic system. In names the first locant of an '*E/Z*' system or of an axial stereogenic unit ('*M/P*' system) is cited. Compound locants (see P-14.3 and P-31.1.4.2) are used when the locants of an individual double bond differ from more than one unit.



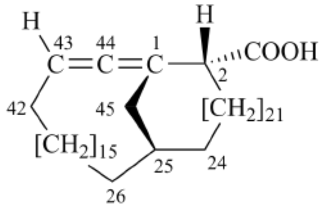
(1*Z*,26*R*)-bicyclo[24.20.1]heptatetraconta-1,2,3-triene (PIN)



[1(44)*E*,2*S*,26*R*]-bicyclo[24.20.1]heptatetraconta-1(46),44,45-trien-2-ol (PIN)



(1*P*,25*R*)-bicyclo[23.19.1]pentatetraconta-1,2-diene (PIN)



[1(43)*P*,2*R*,25*R*]-bicyclo[23.19.1]pentatetraconta-1(44),43-diene-2-carboxylic acid (PIN)

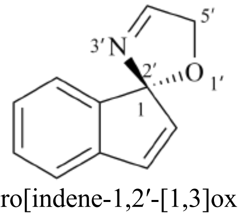
P-93.5.3 Spiro compounds

P-93.5.3.1 Specification of stereogenic spiro atoms of the type ‘Xabcd’, where ‘a’ > ‘b’ > ‘c’ > ‘d’
P-93.5.3.2 Specification of stereogenic spiro atoms of the type ‘Xabab’, where ‘a’ > ‘b’
P-93.5.3.3 Specification of double bonds
P-93.5.3.4 Specification of nontetrahedral stereogenic centers
P-93 5.3.5 Axial chirality of spiro compounds

P-93.5.3.1 Specification of stereogenic spiro atoms of the type ‘Xabcd’, where ‘a’ > ‘b’ > ‘c’ > ‘d’

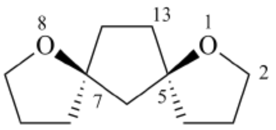
The stereodescriptors ‘*R*’ and ‘*S*’ are used when the spiro atom ‘X’ is surrounded by four atoms arranged as ‘a > b > c > d’. These stereodescriptors are preferred to ‘*cis*’ and ‘*trans*’ that can be used to describe the relative configuration of rings in dispiro compounds. The configuration of any chirality centers located on the spiro skeleton is described by stereodescriptors ‘*R*’ and ‘*S*’ by using the usual method.

Example 1:



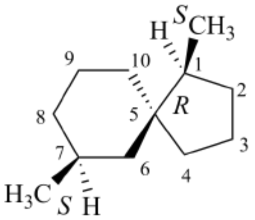
(1*R*)-5′*H*-spiro[indene-1,2′-[1,3]oxazole] (PIN)

Example 2:



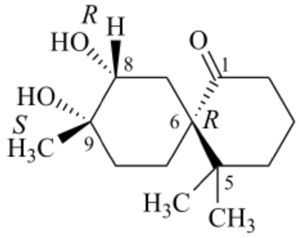
(5*R*,7*S*)-1,8-dioxadispiro[4.1.4^{7}.2^{5}]tridecane (PIN)
cis-1,8-dioxadispiro[4.1.4^{7}.2^{5}]tridecane
(the stereodescriptors ‘*cis*’ and ‘*trans*’ are used here by analogy with disubstituted monocycles described in P-93.5.1.2)

Example 3:

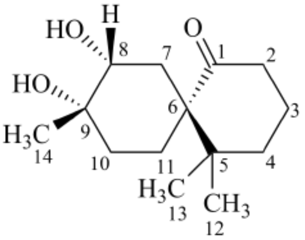

S
H
CH3
1
2
3
4
R
5
6
7
8
9
10
H3C
S
H

(1*S*,5*R*,7*S*)-1,7-dimethylspiro[4.5]decane (PIN)

Example 4:


R
H
HO
8
O
1
HO
S
H3C
9
6
R
5
H3C
CH3

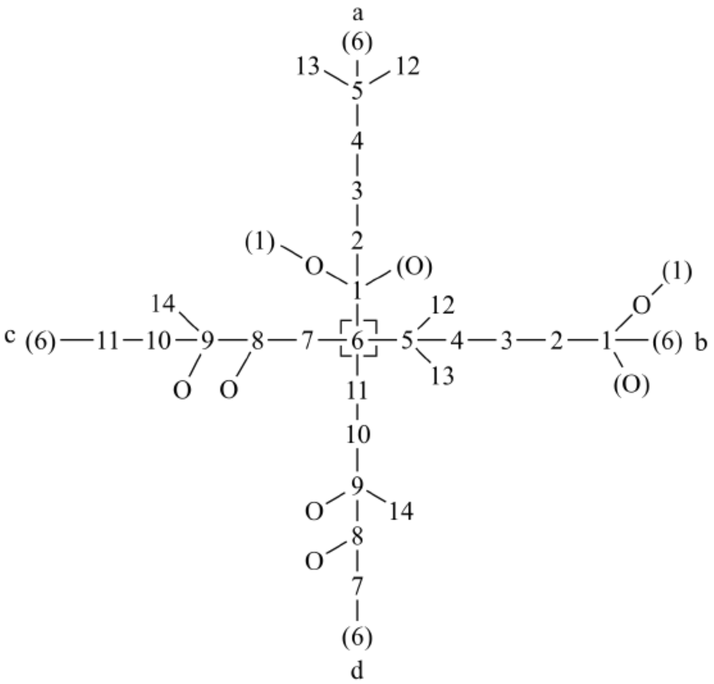
numbering for naming


HO
H
8
7
O
1
2
HO
6
3
H3C
14
9
10
11
5
4
H3C
13
CH3
12

numbering for the simplified digraph

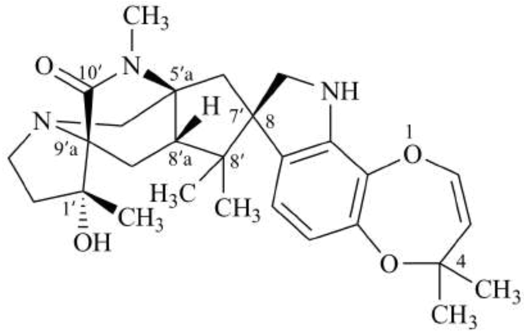
(6*R*,8*R*,9*S*)-8,9-dihydroxy-5,5,9-trimethylspiro[5.5]undecan-1-one (PIN)

Explanation:


a
(6)
13
5
12
4
3
2
(1)
O
1
(O)
c
(6)
11
10
9
14
8
7
6
5
12
13
4
3
2
1
O
(1)
(6)
b
O
O
(O)
11
10
9
O
14
8
O
7
(6)
d

simplified digraph

Example 5:

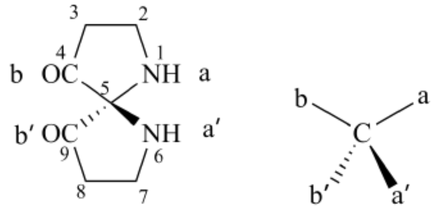

CH3
O
10′
N
5′a
NH
H
7′
8
N
9′a
8′a
8′
1
O
H3C
CH3
1′
CH3
OH
O
4
CH3
CH3

(1′*R*,5′a*S*,7′*R*,8′a*S*,9′a*R*)-1′-hydroxy-1′,4,4,8′,8′,11′-hexamethyl-2′,3′,8′a,9,9′,10-hexahydro-1′*H*,4*H*,5′*H*,6′*H*,8′*H*-spiro[[1,4]dioxepino[2,3-*g*]indole-8,7′-[5a,9a](azanomethano)cyclopenta[*f*]indolizin]-10′-one (PIN)

P-93.5.3.2 Specification of spiro atoms of the type ‘Xabab’, where ‘a’ > ‘b’

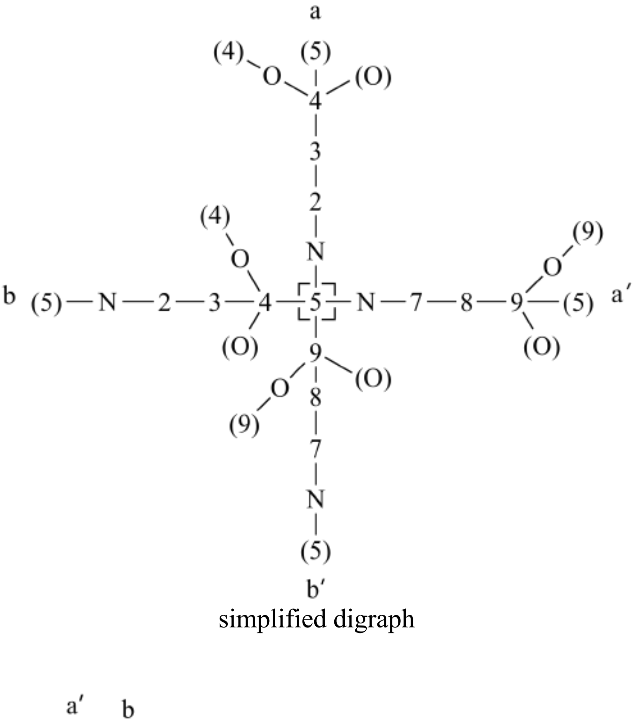
The general methodology used to specify the central configuration of such systems is illustrated below.

Example 1:


3
2
4
1
b
OC
NH
a
5
b′
OC
NH
a′
9
6
8
7
b
a
C
b′
a′

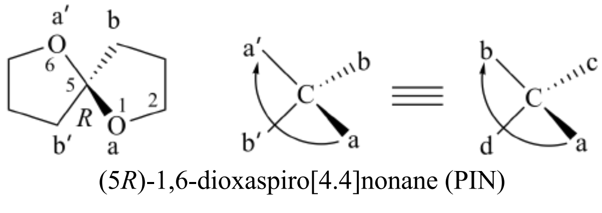
(5*R*)-1,6-diazaspiro[4.4]nonane-4,9-dione (PIN)

Explanation: In this example (see 2.5, ref. 34), the analysis to determine the order of ligands amongst equivalent pairs ‘a’/‘a″ and ‘b’/‘b″, where ‘a’ > ‘b’, starts at the nitrogen atom numbered 1, then goes to the nitrogen atom numbered 6; they are ranked ‘a’ and ‘a″, respectively. The next ligand must be chosen between ‘b’ and ‘b″; as shown in the digraph below, that branch is chosen that contains the nitrogen atom first chosen, i.e. ‘a’ that has precedence over ‘a″; this choice leads the carbon atoms to be ranked as ‘b’ > ‘b″. The configuration ‘*R*’ at the spiro atom ‘C-5’ is determined by using the sequence a > a′ > b > b′.


a
(4)
(5)
O
(O)
4
3
2
(4)
N
(9)
O
O
b
(5)—N—2—3—4—5—N—7—8—9—(5)
a′
(O)
(O)
9
(O)
O
8
(9)
7
N
(5)
b′

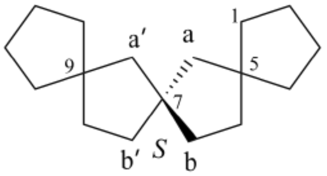
simplified digraph

Example 2:


a′
b
O
6
5
1
2
R
O
b′
a
a′
C
b
b′
a
≡
b
C
c
d
a

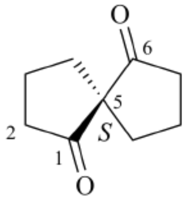
(5*R*)-1,6-dioxaspiro[4.4]nonane (PIN)

Example 3:



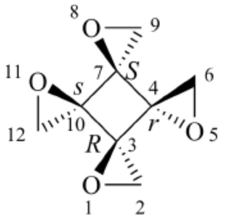
(7*S*)-trispiro[4.1.1.4^{9}.2^{7}.2^{5}]heptadecane (PIN)

Example 4:



(5*S*)-spiro[4.4]nonane-1,6-dione (PIN)

Example 5:



(3*R*,4*r*,7*S*,10*s*)-1,5,8,11-tetraoxatetraspiro[2.0.2^{4}.0.2^{7}.0.2^{10}.0^{3}]dodecane (PIN)
1*r*,5*c*,8*c*,11t-tetraoxatetraspiro[2.0.2^{4}.0.2^{7}.0.2^{10}.0^{3}]dodecane

Note: In this example, stereogenic and pseudoasymmetric centers are present. Application of Sequence Rules **4** and **5** are necessary.

Explanation:

(a) configurations at ‘C-3’ and ‘C-7’ are determined by using Sequence Rule **4**, *like* precedes *unlike*, in accordance with the methodology described in P-92.5;

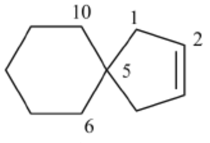
(b) configurations at ‘C-4’ and ‘C-10’ are determined by using Sequence Rule **5**, ‘R_0’ precedes ‘S_0’, in accordance with the methodology described in P-92.6.

(c) the numbering is chosen that gives a ‘*cis*’ attachment at the first point of difference; see P-14.4 (j); thus ‘1*r*,5*c*,8*c*,11*t*’, not ‘1*r*,5*t*,8*c*,11*c*’;

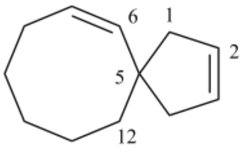
P-93.5.3.3 Specification of double bonds

No stereodescriptor ‘*E*’ or ‘*Z*’ is needed to describe a double bond when the stereogenic unit is located in a ring having less than eight members. All stereodescriptors are used when a larger ring is present.

Examples:



spiro[4.5]dec-2-ene (PIN)

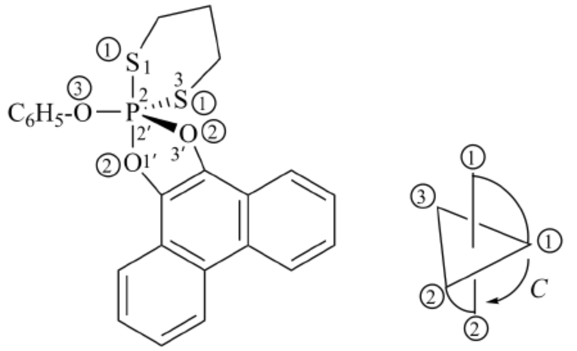


(2*Z*,6*Z*)-spiro[4.7]dodeca-2,6-diene (PIN)
(6*Z*)-spiro[4.7]dodeca-2,6-diene

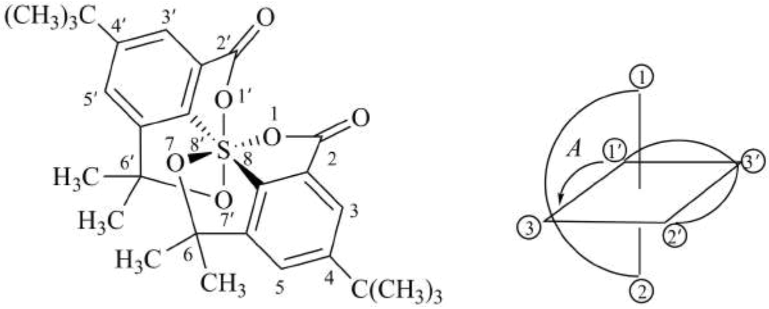
P-93.5.3.4 Specification of nontetrahedral stereogenic centers

As described in P-93.3.4.2, stereodescriptors ‘*A*’ and ‘*C*’, used in coordination chemistry, describe the relative and the absolute configuration of spiro compounds with λ^4, λ^5, and λ^6-hetero spiro atoms.

Examples:



(*TBPY*-5-12-*C*)-2-phenoxy-2*H*-2λ^5-spiro[[1,3,2]dithiaphosphinane-2,2′-phenanthro[9,10-*d*][1,3,2]dioxaphosphole] (PIN)

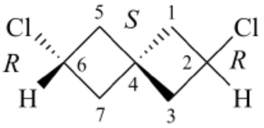


(*OC*-6-22′-*A*)-4,4′-di-*tert*-butyl-6,6,6′,6′-tetramethyl-2*H*,2′*H*,6*H*,6′*H*-8λ^6,8′-spirobi[[1,2]oxathiolo[4,3,2-*hi*][2,1]benzoxathiole]-2,2′-dione (PIN); (see P-93.3.3.7)

P-93.5.3.5 Axial chirality of spiro compounds

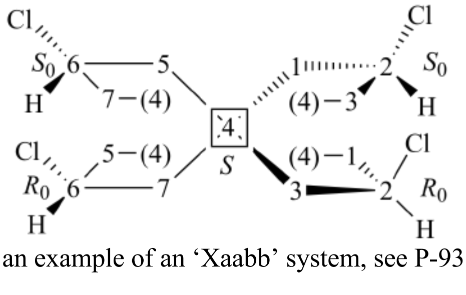
The stereodescriptors '*M*' and '*P*' are used to describe axial chirality of spiro compounds. The sterodescriptors '*R*' and '*S*' can also be used to describe the chirality centers that are present. Sterodescriptors '*R*' and '*S*' are used in preferred IUPAC names.

Example 1:

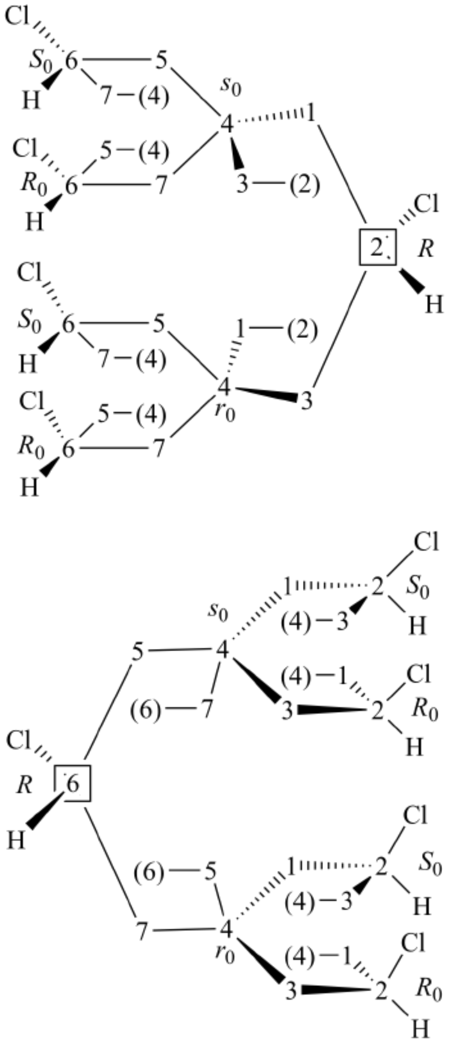


(2*R*,4*S*,6*R*)-2,6-dichlorospiro[3.3]heptane (PIN)
(2*P*)-2,6-dichlorospiro[3.3]heptane

Explanation:

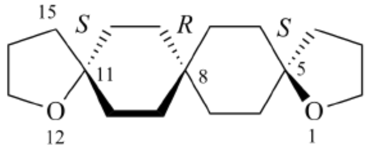


This is an example of an 'Xaabb' system, see P-93.5.3.2.


Cl
S_0
6
5
H
7−(4)
s_0
4
1
Cl
5−(4)
R_0
6
7
3−(2)
H
2
Cl
R
H
Cl
S_0
6
5
1−(2)
H
7−(4)
4
r_0
3
Cl
5−(4)
R_0
6
7
H
Cl
1
2
S_0
s_0
(4)−3
H
5
4
(4)−1
Cl
(6)−7
3
2
R_0
H
Cl
R
6
H
Cl
(6)−5
1
2
S_0
(4)−3
H
7
4
r_0
(4)−1
Cl
3
2
R_0
H

simple digraphs

Example 2:


15
S
R
S
11
8
5
O
O
12
1

(5*S*,8*R*,11*S*)-1,12-dioxatrispiro[4.2.2.4^{11}.2^{8}.2^{5}]nonadecane (PIN)
(5*M*)-1,12-dioxatrispiro[4.2.2.4^{11}.2^{8}.2^{5}]nonadecane

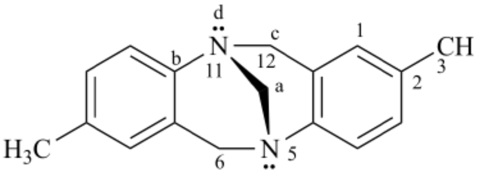
P-93.5.4 Fused and bridged fused compounds

P-93.5.4.1 Specification of configuration by CIP stereodescriptors
P-93.5.4.2 The descriptors ‘*cisoid*’ and ‘*transoid*’

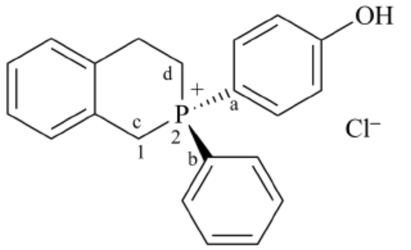
P-93.5.4.1 Specification of configuration by CIP stereodescriptors

A great variety of fused and bridged fused carbocyclic and heterocyclic compounds are described by specifying their stereogenic units as ‘*R*’, ‘*S*’, ‘*r*’, ‘*s*’, ‘*M*’, and ‘*P*’. A few examples illustrate chirality associated with carbon and heteroatoms.

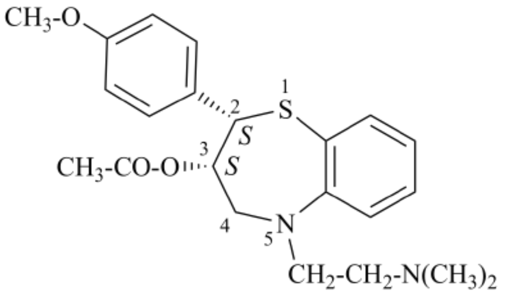
Examples:


d
N
c
1
CH
3
b
11
12
a
2
H$_3$C
6
N
5

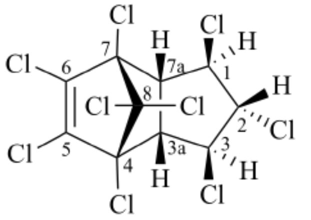
(5*S*,11*S*)-2,8-dimethyl-5,11-6*H*,12*H*-methanodibenzo[*b*,*f*][1,5]diazocine (PIN)


OH
d
+
P
a
c
2
1
b
Cl⁻

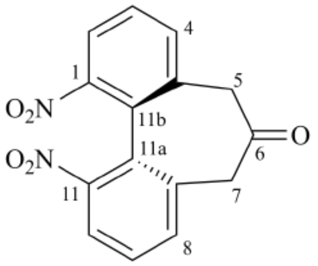
(2*S*)-2-(4-hydroxyphenyl)-2-phenyl-1,2,3,4-tetrahydroisophosphinolin-2-ium chloride (PIN)


CH₃-O
1
S
2
S
3
S
CH₃-CO-O
4
5
N
CH₂-CH₂-N(CH₃)₂

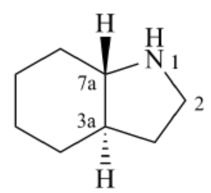
(2*S*,3*S*)-5-[2-(dimethylamino)ethyl]-2-(4-methoxyphenyl)-4-oxo-2,3,4,5-tetrahydro-1,5-benzothiazepin-3-yl acetate (PIN)


Cl
Cl
H
Cl
H
6
7
7a
1
H
Cl
8
Cl
2
Cl
Cl
5
4
3a
3
H
H
Cl
Cl

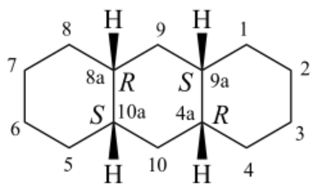
(1*R*,2*r*,3*S*,3a*R*,4*S*,7*R*,7a*S*)-1,2,3,4,5,6,7,8,8-nonachloro-2,3,3a,4,7,7a-hexahydro-1*H*-4,7-methanoindene (PIN)


4
1
5
O₂N
11b
O
11a
6
O₂N
11
7
8

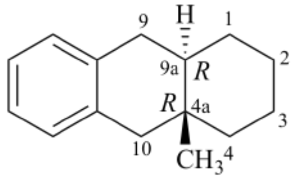
(11a*M*)-1,11-dinitro-5,7-dihydro-6*H*-dibenzo[*a*,*c*][7]annulen-6-one (PIN)
(11a*R*ₐ)-1,11-dinitro-5,7-dihydro-6*H*-dibenzo[*a*,*c*][7]annulen-6-one


H
H
N
1
7a
2
3a
H

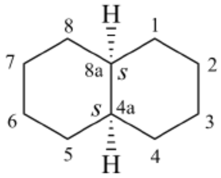
(3a*R*,7a*S*)-octahydro-1*H*-indole (PIN)
trans-octahydroindole


8
H
9
H
1
7
8a
R
S
9a
2
S
10a
4a
R
6
3
5
H
10
H
4

(4a*R*,8a*R*,9a*S*,10a*S*)-tetradecahydroanthracene (PIN)

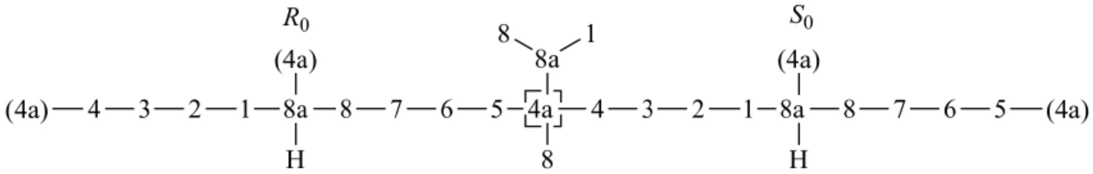

9
H
1
9a
R
2
R
4a
3
10
CH₃
4

(4a*R*,9a*R*)-4a-methyl-1,2,3,4,4a,9,9a,10-octahydroanthracene (PIN)

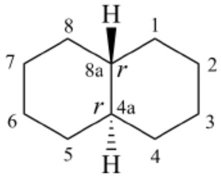

H
8
1
7
8a
s
2
s
4a
6
3
5
H
4

(4a*s*,8a*s*)-decahydronaphthalene (PIN)
cis-decahydronaphthalene

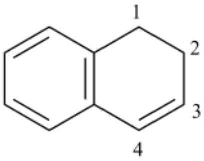
Explanation:


R_0
(4a)
8
1
8a
S_0
(4a)
(4a)—4—3—2—1—8a—8—7—6—5—4a—4—3—2—1—8a—8—7—6—5—(4a)
H
8
H

simplified digraph showing configuration '*s*' at position '4a'


H
8
1
7
8a
r
2
r
4a
6
3
5
H
4

(4a*r*,8a*r*)-decahydronaphthalene (PIN)
trans-decahydronaphthalene



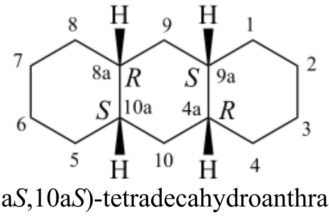
1,2-dihydronaphthalene (PIN)
(the double bond at 'C-3' is not specified as '*Z*'; see P-93.5.1.4.1)

P-93.5.4.2 The descriptors '*cisoid*' and '*transoid*'

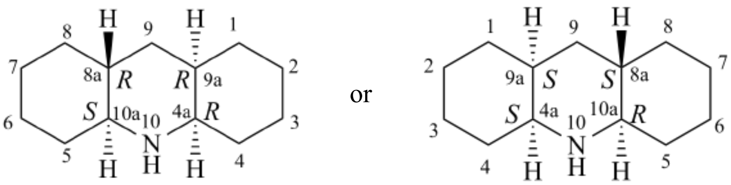
Steric relations at more than one pair of saturated fusion atoms in a fused system are denoted by '*cis*' and '*trans*', each followed by a hyphen, and, if necessary, the corresponding locant of the lower-numbered fusion atom and a second hyphen, all placed before the name of the ring system. Steric relations between the nearest atoms of *cis* or *trans* fusion pairs have been described by descriptors '*cisoid*' or '*transoid*' followed by a hyphen and, when required, the corresponding locants and a second hyphen, the whole placed between the designations of the '*cis*' or '*trans*' junctions concerned. The term 'nearest atom' denotes those atoms linked together through the smallest number of atoms, irrespective of the numbering of the system. When a choice remains between nearest atoms, the pair containing the lower numbered atom is selected.

The descriptors '*cisoid*' and '*transoid*' are not abbreviated. These descriptors are no longer recommended. The notation '*R*' and '*S*', with the descriptor '*rel*' is used instead for describing an enantiomer whose relative configuration only is known.

Examples:


H
H
8
9
1
7
8a
R
S
9a
2
S
10a
4a
R
6
3
5
H
10
H
4

(4a*R*,8a*R*,9a*S*,10a*S*)-tetradecahydroanthracene (PIN)
cis-*cisoid*-*cis*-tetradecahydroanthracene
(this compound is achiral)


H
8
9
H
1
7
8a
R
R
9a
2
S
10a
10
4a
R
6
N
3
5
H
H
H
4
or
1
H
9
H
8
2
9a
S
S
8a
7
S
4a
10
10a
R
3
N
6
4
H
H
H
5

rel-(4a*R*,8a*R*,9a*R*,10a*S*)-tetradecahydroacridine (PIN)
cis-4a-*cisoid*-4a,10a-*trans*-10a-tetradecahydroacridine

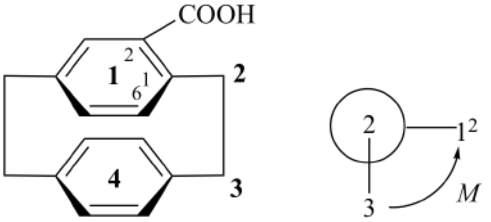
P-93.5.5 Cyclophanes

P-93.5.5.1 Specification of stereogenic planes
P-93.5.5.2 Specification of chirality centers
P-93.5.5.3 Specification of double bonds

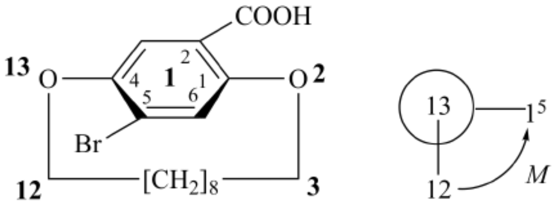
P-93.5.5.1 Specification of stereogenic planes

The descriptors ‘*P*’ and ‘*M*’ are preferred to ‘*R*$_{\mathrm{p}}$’ and ‘*S*$_{\mathrm{p}}$’, respectively, to denote the stereogenic plane in accordance with the methodology described in P-92.1.2.1.3 and P-92.1.2.2.2. When there is a choice of ligands to determine the sense of chirality, the highest ranking in the CIP priority system is selected as reference. In cyclophanes, the composite locant of the ring or ring system that is viewed from the pilot atom is selected as locant to denote the stereogenic unit; this locant is placed at the front of the stereodescriptor.

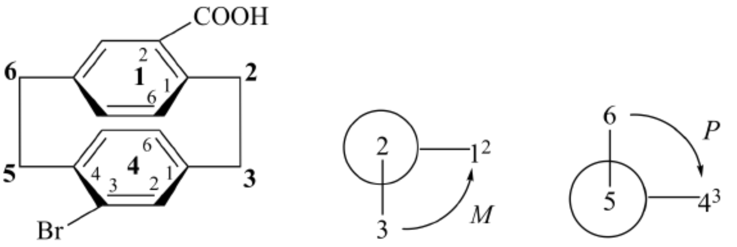
Examples:



(1^{1}*M*)-1,4(1,4)-dibenzenacyclohexaphane-1^{2}-carboxylic acid (PIN)
(1^{1}*S*$_{\mathrm{p}}$)-1,4(1,4)-dibenzenacyclohexaphane-1^{2}-carboxylic acid



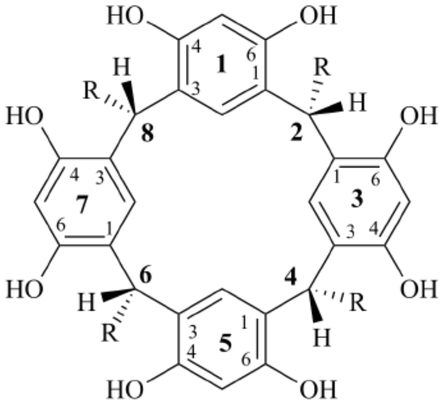
(1^{4}*M*)-1^{5}-bromo-2,13-dioxa-1(1,4)-benzenacyclotridecaphane-1^{2}-carboxylic acid
(1^{4}*S*$_{\mathrm{p}}$)-1^{5}-bromo-2,13-dioxa-1(1,4)-benzenacyclotridecaphane-1^{2}-carboxylic acid
(1*M*)-17-bromo-2,13-dioxabicyclo[12.2.2]octadeca-1(16),14,17-triene-15-carboxylic acid (PIN)



(1^{1}*M*,4^{4}*P*)-4^{3}-bromo-1,4(1,4)-dibenzenacyclohexaphane-1^{2}-carboxylic acid (PIN)
(1^{1}*S*$_{\mathrm{p}}$,4^{4}*R*$_{\mathrm{p}}$)-4^{3}-bromo-1,4(1,4)-dibenzenacyclohexaphane-1^{2}-carboxylic acid

P-93.5.5.2 Specification of chirality centers

Example:



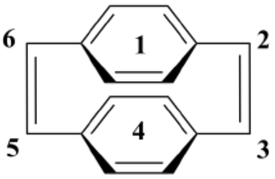
R = –CH$_2$-[CH$_2$]$_7$-CH$_3$

(2*r*,4*r*,6*r*,8*r*)-2,4,6,8-tetranonyl-1,3,5,7(1,3)-tetrabenzenacyclooctaphane-1^{4},1^{6},3^{4},3^{6},5^{4},5^{6},7^{4},7^{6}-octol (PIN)
2*r*,4*c*,6*c*,8*c*-tetranonyl-1,3,5,7(1,3)-tetrabenzenacyclooctaphane-1^{4},1^{6},3^{4},3^{6},5^{4},5^{6},7^{4},7^{6}-octol

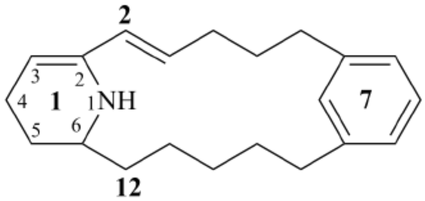
P-93.5.5.3 Specification of double bonds

The omission of stereodescriptors ‘*E*’ and ‘*Z*’ to denote the configuration of double bonds in cyclophanes is related to the total number of nodes in the system; for up to seven nodes, no descriptor is necessary. When more than seven nodes are present, all descriptors of double bonds in rings of more than seven nodes are cited (see P-91.2.2).

Examples:



1,4(1,4)-dibenzenacyclohexaphane-2,5-diene (PIN)



(2*E*)-1^1,1^4,1^5,1^6-tetrahydro-1(2,6)-pyridina-7(1,3)-benzenacyclododecaphan-2-ene (PIN)

P-93.5.6 Fullerenes

P-93.5.6.1 Definitions and general methodology

Only general principles for describing stereochemical configuration of fullerenes are discussed briefly and exemplified in this section. Describing stereochemical configuration of fullerenes is extremely complex because of different factors such as the numbering of the fullerene molecule, systematic or trivial (in these recommendations, only the systematic numbering given in refs. 10, 11 is used), the nature and disposition of substituent groups on the fullerene, and the plurality of stereodescriptors necessary to describe their stereochemical configuration fully. For a full discussion of the description of fullerene configuration, one must go to the original publication (Section 17 in ref. 10).

For the purpose of describing stereochemical configuration, fullerenes and their derivatives are classified into four types depending on the origin of their chirality:

P-93.5.6.2 Type 1. Inherently chiral parent fullerenes;
P-93.5.6.3 Type 2. Substituted fullerenes inherently chiral because of their substitution pattern;
P-93.5.6.4 Type 3. Substituted fullerenes noninherently chiral because of their substitution pattern;
P-93.5.6.5 Type 4. Chirality due to chiral substituents;
P-93.5.6.6 Superimposition of stereogenic elements in a fullerene molecule

The four types are classified by the ‘substitution test’ that consists of changing the substituents in a single fullerene unit into a ‘achiral test substituent’, ‘T’, and verifying the chirality of the fullerene so modified by the presence of ‘T’ substituents (see Fig. 9.2)

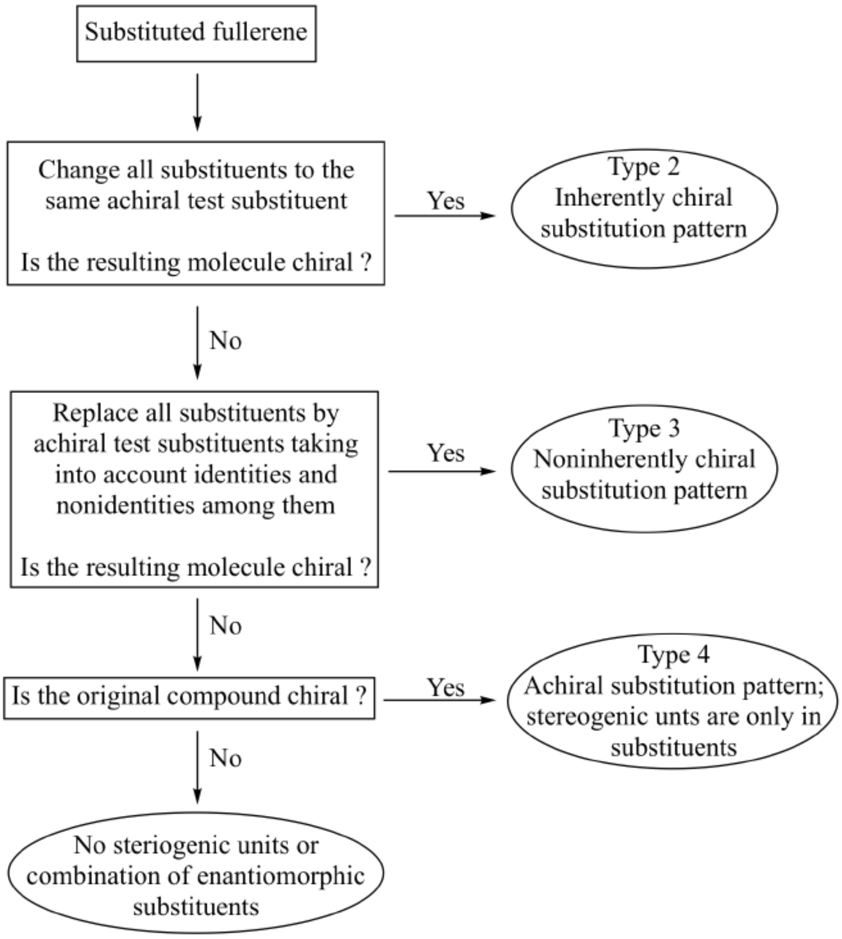
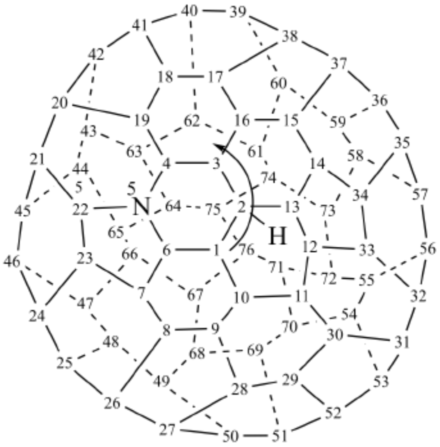

Substituted fullerene
Change all substituents to the same achiral test substituent
Is the resulting molecule chiral ?
Yes
Type 2
Inherently chiral substitution pattern
No
Replace all substituents by achiral test substituents taking into account identities and nonidentities among them
Is the resulting molecule chiral ?
Yes
Type 3
Noninherently chiral substitution pattern
No
Is the original compound chiral ?
Yes
Type 4
Achiral substitution pattern; stereogenic unts are only in substituents
No
No steriogenic units or combination of enantiomorphic substituents

Fig. 9.2 Classification of fullerene chirality by a stepwise substitution pattern

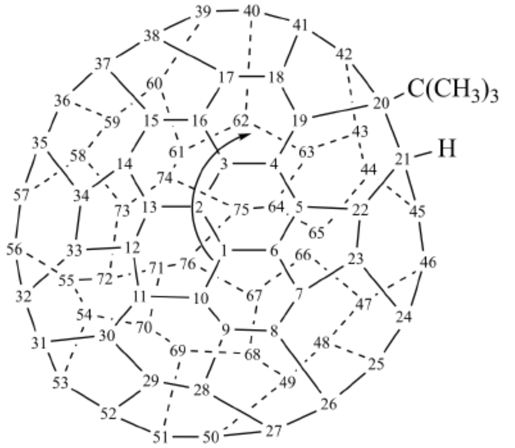
P-93.5.6.2 Type 1. Inherently chiral parent fullerenes.

The two fullerene molecules described in Section P-27, (C_{60}-I_h)[5,6]fullerene and the (C_{70}-$D_{5h(6)}$)[5,6]fullerene, are achiral; they are not inherently chiral. In contrast, the (C_{76}-D_2)[5,6]fullerene shown below is inherently chiral. The numbering of an inherently chiral fullerene applies to a specific enantiomer; the other enantiomer has a numbering that is the mirror-image of the first numbering. A description of the handedness of the numbering scheme is sufficient to characterize the absolute configuration of the fullerene unambiguously. The viewer, looking at the polygon in which the numbering starts from outside the fullerene cage, traces a path from 'C-1' to 'C-2' to 'C-3', which is never aligned in a fullerene structure. If this path describes a clockwise direction, the configuration is indicated by the stereodescriptor '${}^{f,x}C$', where the superscript 'f' indicates that the descriptor refers to a fullerene, and the superscript 'x' is either '*s*' for the systematic numbering or 't' for the trivial numbering described in P-27.3. If the path from 'C-1' to 'C-2' to 'C-3' describes an anticlockwise direction, the descriptor is '${}^{f,x}A$'. Thus, the fullerene on the right hand side below is described by the stereodescriptor '${}^{f,s}C$'; its name is (${}^{f,s}C$)-(C_{76}-D_2)[5,6]fullerene. The fullerene on the left hand side is (${}^{f,s}A$)-(C_{76}-D_2)[5,6]fullerene. The systematic numbering of these fullerenes is that used by Chemical Abstracts Service (ref. 22).

Examples:



I



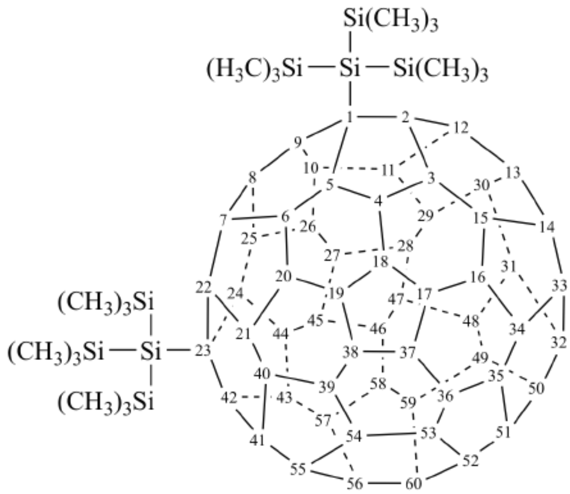
II

I (${}^{f,s}A$)-2*H*-5-aza-(C_{76}-D_2)[5,6]fullerene (PIN)
II (${}^{f,s}C$)-20-*tert*-butyl-20,21-dihydro(C_{76}-D_2)[5,6]fullerene (PIN)

P-93.5.6.3 Type 2. Substituted fullerenes inherently chiral because of their substitution pattern.

Derivatives of achiral (and chiral) parent fullerenes in which the presence of substituents, chiral or achiral, identical or different, on the fullerene skeleton creates a chiral substitution pattern are said to have an inherently chiral substitution pattern. Fullerene compounds of this type are all substituted achiral fullerenes. They have an inherently chiral substitution pattern if the existence of enantiomers is inherent to the geometrical arrangement of the substitution sites on the fullerene parent regardless of whether the substituents are identical or different. In these fullerene derivatives there is a unique numbering scheme that leads to the lowest set of locants for the substituents. As in P-93.5.6.2, the stereodescriptors are‘$^{\mathrm{f,x}}C$’ and ‘$^{\mathrm{f,x}}A$’.

Example:



($^{\mathrm{f,s}}C$)-1,23-bis[1,1,1,3,3,3-hexamethyl-2-(trimethylsilyl)trisilan-2-yl]-1,23-dihydro(C_{60}-I_h)[5,6]-fullerene (PIN)

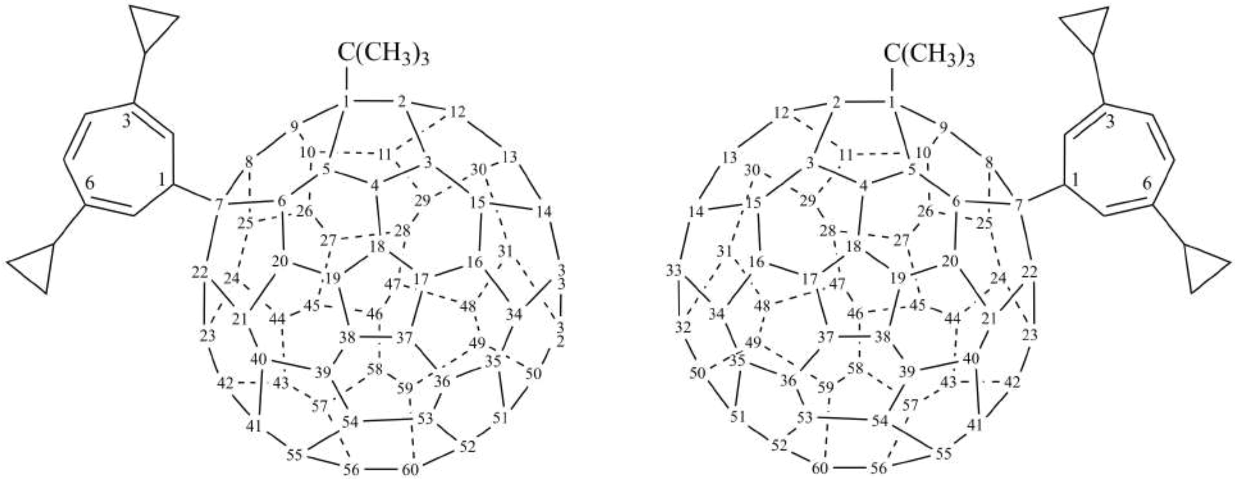
Explanation: Locants for the substituents are ‘1,23’ for clockwise numbering. But for anticlockwise numbering they are ‘1,29’ and since ‘1,23’ is lower that ‘1,29’ according to the principle of lowest locants (see P-14.3.5) and therefore clockwise numbering is preferred. For the enantiomer, the lower locants ‘1,23’ would be obtained on anticlockwise numbering and the descriptor would be ($^{\mathrm{f,s}}A$)-.

P-93.5.6.4 Type 3. Substituted fullerenes noninherently chiral because of their substitution pattern.

Derivatives of achiral parent fullerenes in which a chiral substitution pattern on the fullerene is due only to nonidentities among the substituents have a noninherently chiral substitution pattern.

The CIP system is used to rank substituents according to Sequence Rules **1** or **2** (see P-92.2 and P-92.3). In the following enantiomeric disubstituted fullerenes, the *tert*-butyl group has precedence over the 3,6-dicyclopropylcyclohepta-2,4,6-trien-1-yl group. Stereodescriptors ‘$^{\mathrm{f,x}}C$’ and ‘$^{\mathrm{f,x}}A$’ are used to describe the absolute configuration, as indicated in P-93.5.6.2, in conformity with whether the path C-1 to C-2 to C-3 is clockwise or anticlockwise.

Example:



($^{\mathrm{f,s}}C$)- ($^{\mathrm{f,s}}A$)-

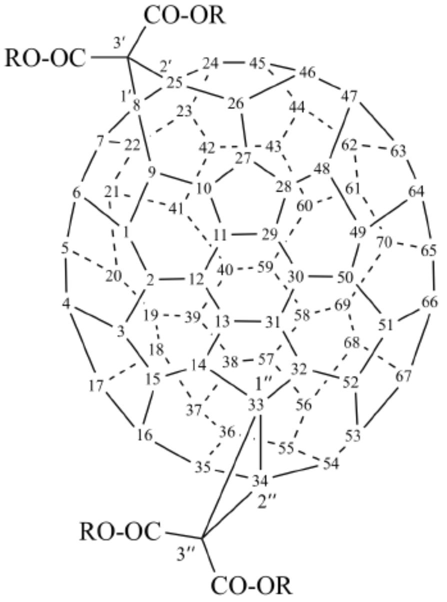
1-*tert*-butyl-7-(3,6-dicyclopropylcyclohepta-2,4,6-trien-1-yl)-1,7-dihydro(C_{60}-I_h)[5,6]fullerene (PIN)

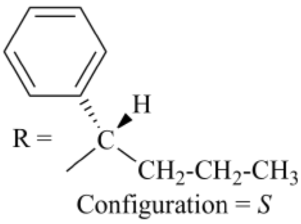
Explanation: This compound is chiral only because the substituents are constitutionally different. The parent fullerene is achiral and it does not have an inherently chiral substitution pattern because replacement of both substituents by the same achiral test substituent, ‘T’, results in an achiral compound. Therefore it has a noninherently chiral substitution pattern. The *tert*-butyl group is assigned the locant ‘1’ because its CIP priority is higher than that of the 3,6-dicyclopropylcyclohepta-2,4,6-trien-1-yl group.

P-93.5.6.5 Type 4. Chirality due to chiral substituents.

Derivatives of achiral parent fullerenes in which the presence of chiral substituents does not create a chiral substitution pattern have the stereogenic units located exclusively in the substituents. In derivatives of this type, the chirality located in substituents is expressed by the usual CIP stereodescriptors. In the following example, the ‘*S*’ configuration for the organyl group present in the –CO-O-R substituents is the only stereodescriptor needed to express the configuration of the compound.

Example:





tetrakis[(1*S*)-1-phenylbutyl] 3′*H*,3″*H*-dicyclopropa[8,25:16,35](C_{70}-$D_{5\mathrm{h}(6)}$)[5,6]fullerene-3′3′,3″,3″-tetracarboxylate (PIN)

Explanations:

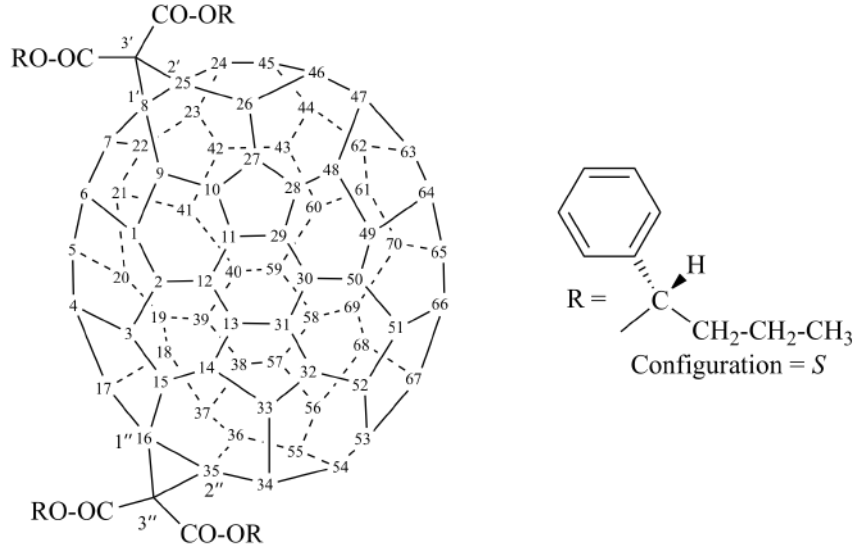
(a) This fullerene derivative is chiral. The parent fullerene is achiral and the derivative has an achiral substitution pattern. The configuration of the substituents can be described by the normal descriptors of organic nomenclature (see P-91.3).

(b) If the esters of the acid in the above example were different, the parent fullerene and its substitution pattern would still be achiral and therefore any chirality of the original compound would be due to stereogenic centers located in the substituents.

P-93.5.6.6 Superimposition of stereogenic elements in a fullerene molecule.

If a fullerene derivative with an inherently or noninherently chiral substitution pattern carries chiral substituents, the configuration of both types of stereogenic elements has to be indicated. The two types are independent of each other and the configuration of both must be specified for a full description of the compound.

Example:



tetrakis[(1*S*)-1-phenylbutyl]
($^{f,s}C$)-3′*H*,3″*H*-dicyclopropa[8,25:33,34]-(C_{70}-$D_{5h(6)}$)[5,6]fullerene-3″3′,3″,3″-tetracarboxylate (PIN)

Explanation: The chiralities of the stereogenic centers in the esters are superimposed on the descriptor for the fullerene with the inherently chiral substitution pattern. The enantiomer would be named:

tetrakis[(1*R*)-1-phenylbutyl] ($^{f,s}A$)-3′*H*,3″*H*-dicyclopropa[8,25:33,34]-(C_{70}-$D_{5h(6)}$)[5,6]fullerene-3′,3′,3″,3″-tetracarboxylate (PIN)

and similarly for the various diastereoisomers.

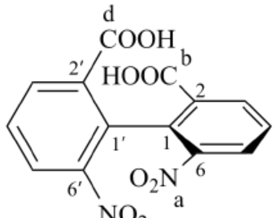
P-93.5.7 Ring assemblies

P-93.5.7.1 Specification of stereogenic axes
P-93.5.7.2 Specification of stereogenic centers
P-93.5.7.3 Specification of double bonds in unsaturated alicyclic rings assemblies

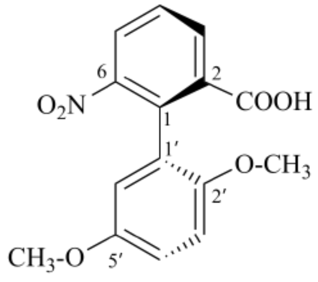
P-93.5.7.1 Specification of stereogenic axes

The descriptors ‘*M*’ and ‘*P*’ are preferred to ‘R_a’ and ‘S_a’, respectively, to denote the stereogenic axis, in accordance with the methodology described in P-92.1.2.2.1 and P-92.1.2.1.2.

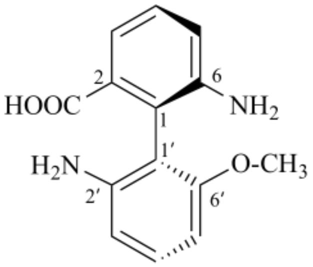
Examples:



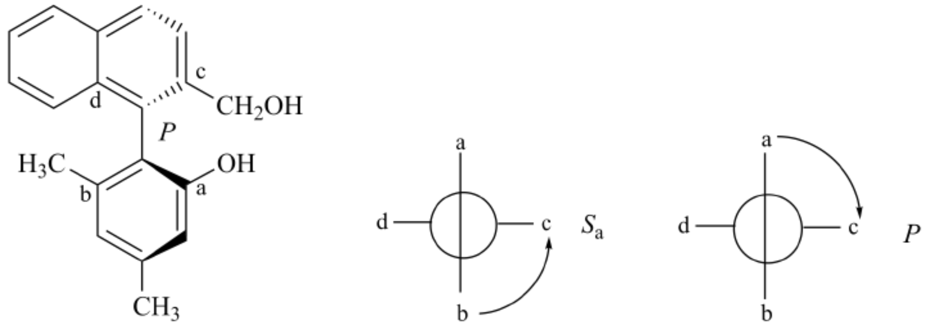
(1*M*)-6,6′-dinitro[1,1′-biphenyl]-2,2′-dicarboxylic acid (PIN)
(1R_a)-6,6′-dinitro[1,1′-biphenyl]-2,2′-dicarboxylic acid



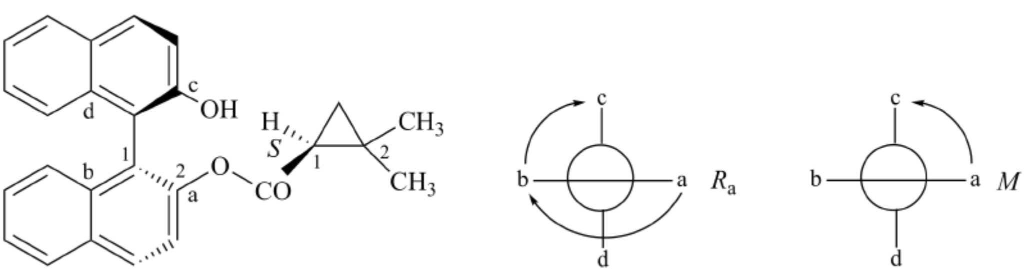
(1*P*)-2′,5′-dimethoxy-6-nitro[1,1′-biphenyl]-2-carboxylic acid (PIN)
(1S_a)-2′,5′-dimethoxy-6-nitro[1,1′-biphenyl]-2-carboxylic acid


HOOC
2
6
NH2
1
1′
H2N
O-CH3
2′
6′

(1*M*)-2′,6-diamino-6′-methoxy[1,1′-biphenyl]-2-carboxylic acid (PIN)
(1*R*a)-2′,6-diamino-6′-methoxy[1,1′-biphenyl]-2-carboxylic acid


c
d
CH2OH
P
H3C
OH
b
a
CH3
a
d
c
Sa
b
a
d
c
P
b

(2*P*)-2-[2-(hydroxymethyl)naphthalen-1-yl]-3,5-dimethylphenol (PIN)
(2*S*a)-2-[2-(hydroxymethyl)naphthalen-1-yl]-3,5-dimethylphenol

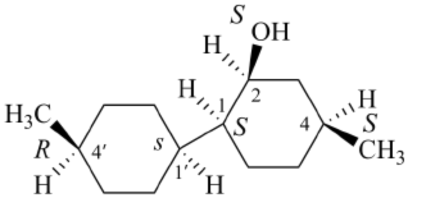

c
d
OH
H
S
1
2
CH3
CH3
1
b
2
O
a
CO
c
b
a
Ra
d
c
b
a
M
d

(1*M*)-2′-hydroxy[1,1′-binaphthalen]-2-yl (1*S*)-2,2-dimethylcyclopropane-1-carboxylate (PIN)
(1*R*a)-2′-hydroxy[1,1′-binaphthalen]-2-yl (1*S*)-2,2-dimethylcyclopropane-1-carboxylate

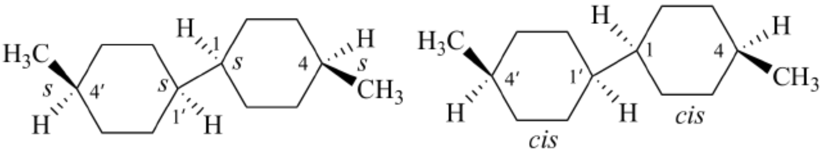
P-93.5.7.2 Specification of stereogenic centers

In preferred IUPAC names, stereogenic centers are specified by stereodescriptors such as '*R*', '*S*,' '*r*', and '*s*'. In general nomenclature, the stereodescriptors '*cis*' and '*trans*' may be used as described in P-93.5.1.2.

Examples:

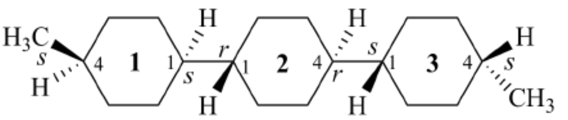

S
OH
H
H
2
1
H
H3C
S
4
S
R
4′
s
CH3
H
1′
H

(1*S*,1′*s*,2*S*,4*S*,4′*R*)-4,4′-dimethyl[1,1′-bi(cyclohexan)]-2-ol (PIN)

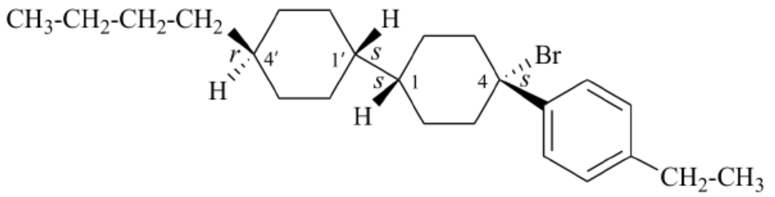

H3C
s
4′
H
s
1′
H
H
1
s
4
H
s
CH3
H3C
4′
H
1′
H
cis
H
1
4
H
CH3
cis

(a)
(b)

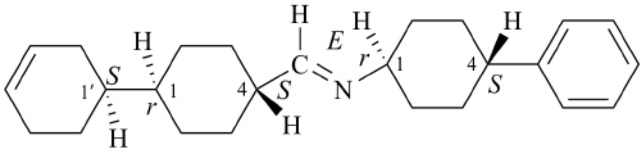
(a) (1*s*,1′*s*,4*s*,4′*s*)-4,4′-dimethyl-1,1′-bi(cyclohexane) (PIN)
(b) [1(4)-*cis*,1′(4′)-*cis*]-4,4′-dimethyl-1,1′-bi(cyclohexane)


H3C
s
H
4
1
1
s
H
r
H
1
2
4
r
H
s
H
1
3
4
H
s
CH3

($1^1s,1^4s,2^1r,2^4r,3^1s,3^4s$)-$1^4,3^4$-dimethyl-$1^1,2^1{:}2^4,3^1$-tercyclohexane (PIN)
[$1^1(1^4)$-*cis*,$2^1(2^4)$-*trans*,$3^1(3^4)$-*cis*]-$1^4,3^4$-dimethyl-$1^1,2^1{:}2^4,3^1$-tercyclohexane



(1^{1}*s*,1^{4}*r*,2^{1}*s*,2^{4}*s*)-2^{4}-bromo-1^{4}-butyl-3^{4}-ethyl-1^{1},1^{2},1^{3},1^{4},1^{5},1^{6},2^{1},2^{2},2^{3},2^{4},2^{5},2^{6}-dodecahydro-1^{1},2^{1}:2^{4},3^{1}-terphenyl (PIN)
(1*s*,1′*s*,4*s*,4′*r*)-4-bromo-4′-butyl-4-(4-ethylphenyl)-1,1′-bi(cyclohexane) [numbering shown]
(1*s*,1′*s*,4*r*,4′*s*)-4′-bromo-4-butyl-4″-ethyl-1,1′,2,2′,3,3′,4,4′,5,5′,6,6′-dodecahydro-1,1′:4′,1″-terphenyl

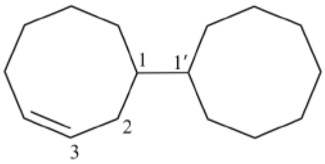


(1*E*)-1-[(1*r*,1′*S*,4*S*)-[1,1′-bi(cyclohexan)]-3′-en-4-yl]-*N*-[(1*r*,4*S*)-4-phenylcyclohexyl]methanimine (PIN)
(*E*)-1-[1(4)-*trans*-(1′*S*)-[1,1′-bi(cyclohexan)]-3′-en-4-yl]-*N*-*trans*-4-phenylcyclohexyl)methanimine

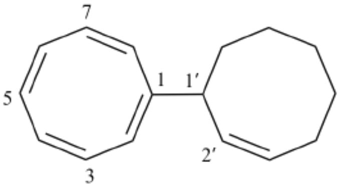
P-93.5.7.3 Specification of double bonds in unsaturated alicyclic ring assemblies

The general methodology described in P-91.2.2 is applied to unsaturated alicyclic ring assemblies. In eight-membered rings, all stereogenic units must be specified, when one needs to be specified.

Examples:



(3*Z*)-[1,1′-bi(cyclooctan)]-3-ene (PIN)

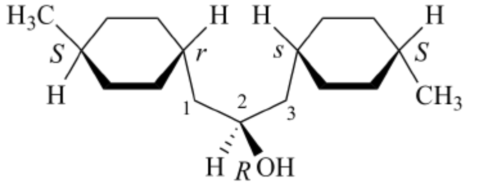


(1*Z*,2′*Z*,3*Z*,5*Z*,7*Z*)-[1,1′-bi(cyclooctane)]-1,2′,3,5,7-pentaene (PIN)

P-93.6 COMPOUNDS COMPOSED OF RINGS AND CHAINS

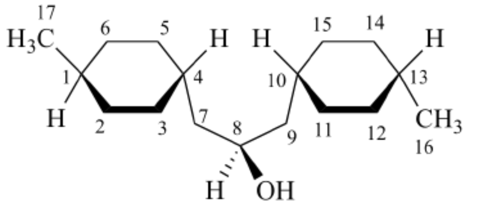
In the construction of names of organic compounds, the first step is to form the name according to the principles, rules, and conventions described in Chapters P-1 through P-8; in a second step, stereodescriptors are added, in accordance with rules expressed in Chapter P-9. This addition of stereodescriptors does not change a preferred IUPAC name, be it a substitutive name, a phane name, or a functional class name, and the corresponding names formed by skeletal ('a') replacement nomenclature, provided that stereodescriptors are added in conformity with numbering. Care must be taken in dealing with multiplicative names which must be formed in accordance with the symmetry requirements, including stereodescriptors, essential to this type of nomenclature for being accepted as preferred IUPAC names.

Example 1:

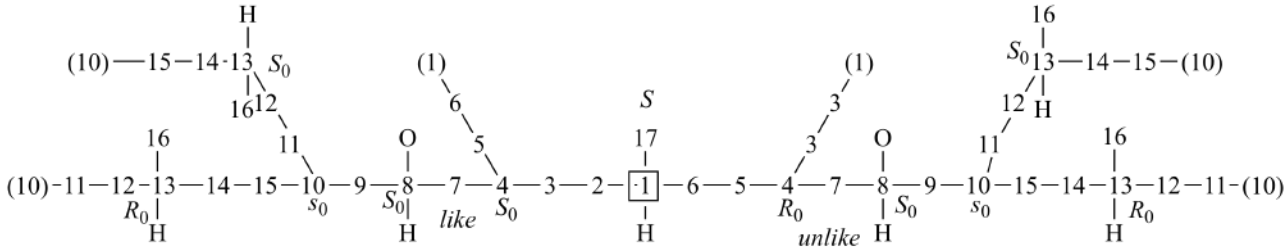


(2*R*)-1-[(1*r*,4*S*)-4-methylcyclohexyl]-3-[(1*s*,4*S*)-4-methylcyclohexyl]propan-2-ol (PIN)
(2*R*)-1-(*cis*-4-methylcyclohexyl)-3-(*trans*-4-methylcyclohexyl)propan-2-ol

Explanation:

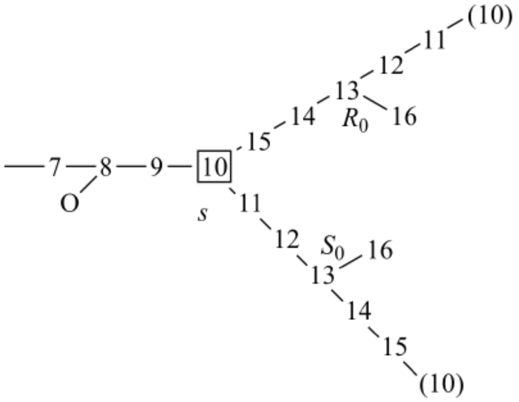


arbitrary numbering for the simplified digraphs



H
(10)—15—14-13 S_0
16 12
11
16
(1)
6
5
O
S
17
(1)
3
3
O
16
S_0 13—14—15—(10)
12 H
11
16
(10)-11—12-13—14—15—10—9—8—7—4—3—2—1—6—5—4—7—8—9—10—15—14—13—12—11-(10)
R_0 H
s_0
S_0 H
like
S_0
H
R_0
unlike
S_0 H
s_0
R_0 H

simplified digraph for the configuration '*S*' at C-1 (sequence rule **4b** *like* > *unlike*)

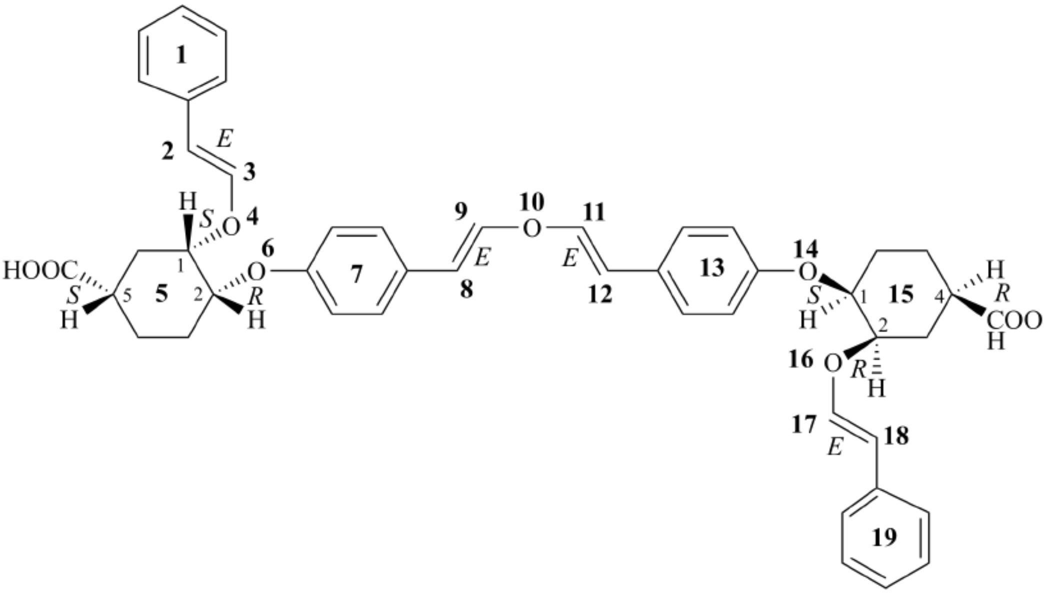


(10)
11
12
13
14 R_0 16
15
—7—8—9—10
O
s
11
12 S_0 16
13
14
15
(10)

partial simplified digraph for the configuration '*s*' at C-10

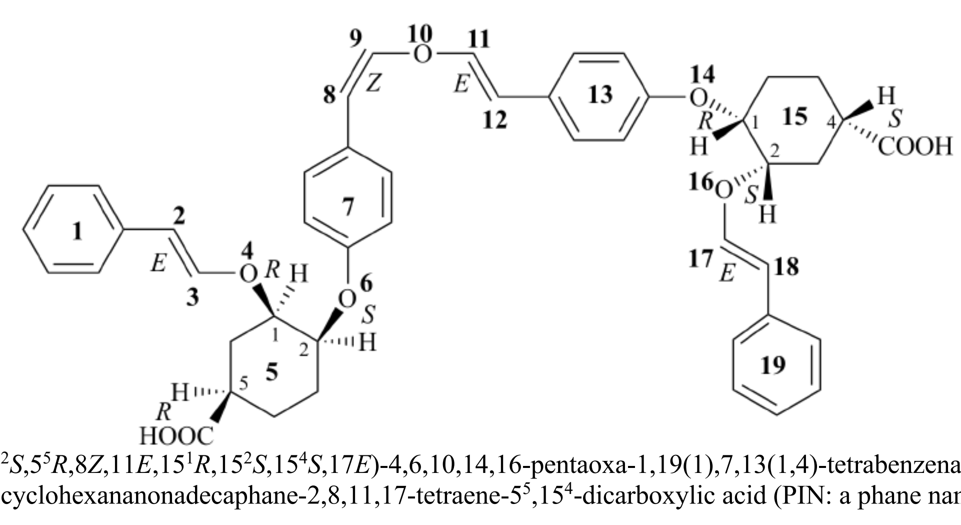
The configuration '*R*' at 'C-8' is determined by applying Sequence Rule **4c**, '*r*' precedes '*s*'.

Example 2:



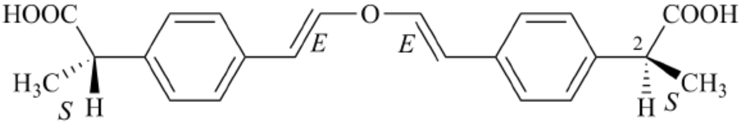
(2*E*,5^1*S*,5^2*R*,5^5*S*,8*E*,11*E*,15^1*S*,15^2*R*,15^4*R*,17*E*)-4,6,10,14,16-pentaoxa-1,19(1),7,13(1,4)-tetrabenzena-5,15(1,2)-dicyclohexananonadecaphane-2,8,11,17-tetraene-5^5,15^4-dicarboxylic acid (PIN: a phane name)

Example 3:



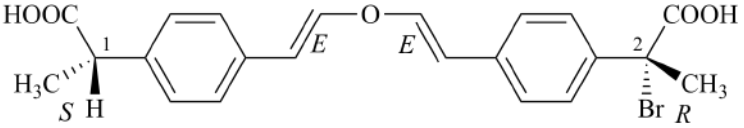
(2*E*,5^1*R*,5^2*S*,5^5*R*,8*Z*,11*E*,15^1*R*,15^2*S*,15^4*S*,17*E*)-4,6,10,14,16-pentaoxa-1,19(1),7,13(1,4)-tetrabenzena-5,15(1,2)-dicyclohexananonadecaphane-2,8,11,17-tetraene-5^5,15^4-dicarboxylic acid (PIN: a phane name)

Example 4:



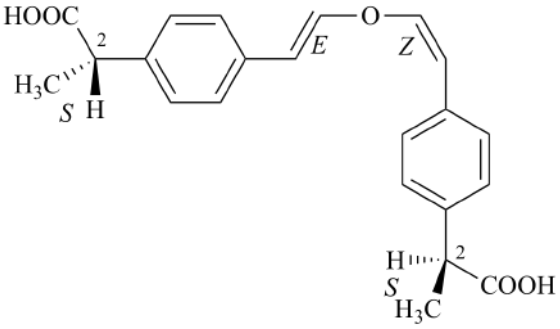
(2*S*,2′*S*)-2,2′-{oxybis[(1*E*)-ethene-2,1-diyl-4,1-phenylene]}dipropanoic acid (PIN)
(a multiplicative name is the preferred IUPAC name, the symmetry requirements for its use being fulfilled)

Example 5:



(2*R*)-2-bromo-2-{4-[(*E*)-2-{[(*E*)-2-{4-[(1*S*)-1-carboxyethyl]phenyl}ethen-1-yl]oxy}ethen-1-yl]phenyl}propanoic acid
(PIN; a multiplicative name is not allowed, because of the different stereodescriptors and
nonidentical repeated parent structures)

Example 6:



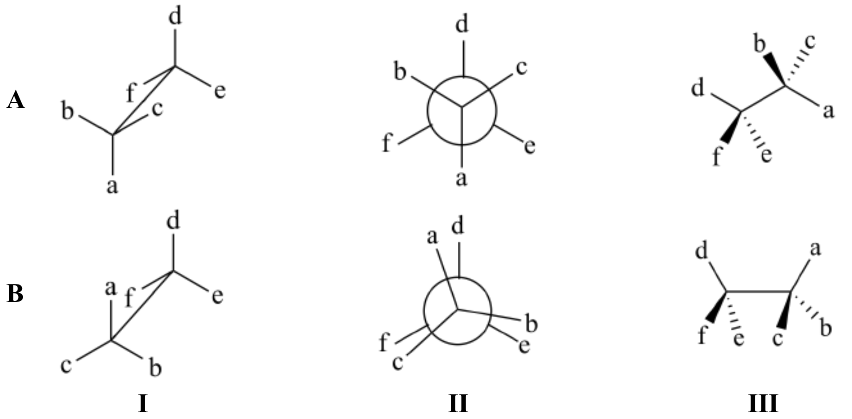
(2*S*)-2-{4-[(*E*)-2-{(*Z*)-2-{4-[(1*S*)-1-carboxyethyl]phenyl}ethen-1-yl]oxy}ethen-1-yl]phenyl}propanoic acid (PIN;
a multiplicative name is not allowed, because of the lack of identical components in the central substituent group)

P-94 CONFORMATION AND CONFORMATIONAL STEREODESCRIPTORS

This Section is based on the IUPAC publication "Basic Terminology of Stereochemistry" (see ref. 37).

P-94.1 DEFINITION

A conformation is the spatial arrangement of the atoms affording distinction between stereoisomers which can be interconverted by rotations about formally single bonds, as exemplified for conformers A and B in Fig. 9.3.



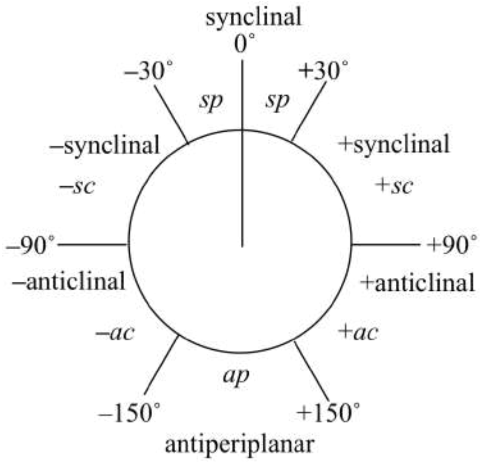
Sawhorse projection
Newman projection
Zig-zag projection

Fig. 9.3. Three different representations of two conformers A and B.

P-94.2 TORSION ANGLE

P-94.2.1 In an assembly of attached atoms X-A-B-Y, where neither X nor Y is collinear with A and B, the smaller angle subtended by the bonds X-A and Y-B in a plane projection obtained by viewing the assembly along the axis A-B is termed the 'torsion angle', denoted by the italicized lower-case Greek letter θ. The torsion angle is considered positive or negative according as the bond atom X or Y requires rotation to the right (clockwise) or left (anticlockwise), respectively, in order that its direction may coincide with that of the bond to the rear selected atom Y or X. The multiplicity of the bonding of the various atoms is irrelevant. A torsion angle also exists if the axis for rotation is formed by a collinear set of more than two atoms directly attached to each other.

Conformations are described as synperiplanar (*sp*), synclinal (*sc*), anticlinal (*ac*), or antiperiplaner (*ap*), according as the torsion angle is within ±30° of 0°; ±60°, ±120°, or ±180°, respectively; the letters in parentheses are the corresponding abbreviations.


synclinal
0°
–30°
+30°
sp
sp
–synclinal
+synclinal
–sc
+sc
–90°
+90°
–anticlinal
+anticlinal
–ac
+ac
ap
–150°
+150°
antiperiplanar

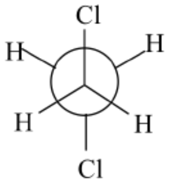
To choose the appropriate stereodescriptor, atoms or groups are selected from each set to define the torsion angle according to the following criteria:

(1) if all the atoms or groups of a set are different, that one of each set that has priority by the sequence rule;

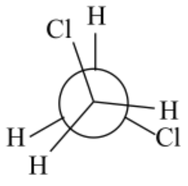
(2) if one of a set is unique, that one;

(3) if all of a set are identical, that one which provides the smallest torsion angle.

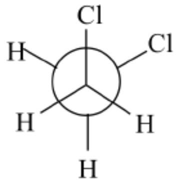
Examples:



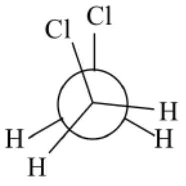
antiperiplanar



anticlinal

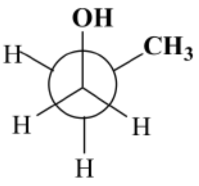


synclinal

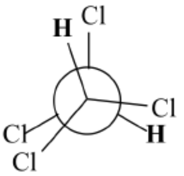


synperiplanar

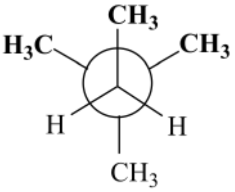
(the two chlorine atoms decide the conformation)



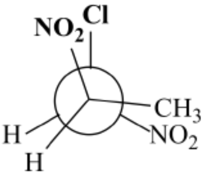
synclinal


H
Cl
Cl
H
Cl
Cl

anticlinal


CH3
H3C
CH3
H
H
CH3

synclinal


NO2
Cl
CH3
NO2
H
H

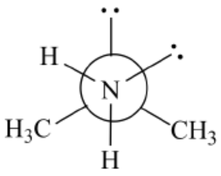
synperiplanar

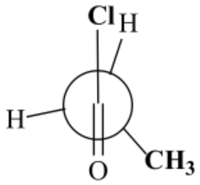
Criteria from above for:

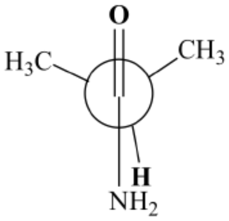
	synclinal	anticlinal	synclinal	synperiplanar
the rear atom	2	2	3	1
the front atom	2	2	2	1

P-94.2.2 If ‘A’ and ‘B’ in ‘X-A-B-Y’ are trigonal centers, a lone pair of electrons represented by two dots is taken into consideration to decide the description of the conformation, as illustrated by the example below describing the conformation of 1,1-dimethylhydrazine, $(CH_3)_2N$-NH_2; the lone pairs of electrons are the phantom atoms of the sequence rules symbolism. Similarly, trigonal centers involving double bonds are analyzed with the sequence rules by using duplicate atoms to determine the order of precedence.

Examples:







	$(CH_3)_2N\text{-}NH_2$	$CH_3\text{-}CH_2\text{-}CO\text{-}Cl$	$(CH_3)_2CH\text{-}CO\text{-}NH_2$
	synclinal	anticlinal	antiperiplanar
Criteria from above for:			
the rear atom			
	2	2	2
the front atom			
	2	1	1

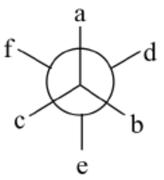
P-94.3 SPECIFIC STEREODESCRIPTORS

Stereodescriptors are used to denote specific conformers, both aliphatic and alicyclic.

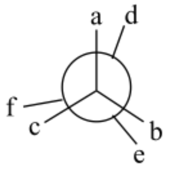
P-94.3.1 Eclipsed, staggered and gauche (or skew) conformations

P-94.3.1.1 Two atoms or groups attached to two adjacent atoms are said to be 'eclipsed' if the torsion angle between them is zero. They are said to be 'staggered' when they are as far apart as possible from an eclipsed conformation. 'Gauche' or 'skew' are synonymous with synclinal, which is preferred. The stereodescriptors '*trans*' or '*anti*' are not recommended in place of 'anticlinal', nor '*cis*' or '*syn*' in place of 'synclinal'. Eclipsed and staggered are stereodescriptors used to denote the conformations when all ligands are identical.

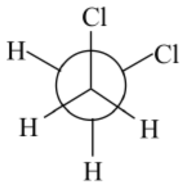
Examples:



staggered conformation
(all the attached groups
are staggered)

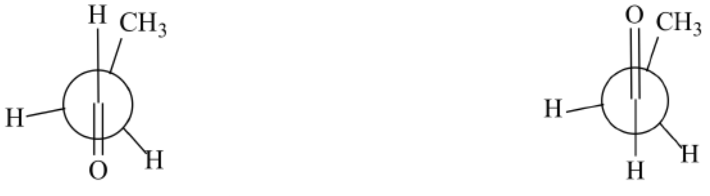


eclipsed conformation
(the pairs a-d, b-e, and
c-f are eclipsed)



synclinal (preferred)
gauche or skew

P-94.3.1.2 For a structure containing the grouping $R_3C\text{-}C(Y){=}X$ (with identical or different R groups) the conformation in which the torsion angle is such that X is antiperiplanar to one of the R group, and, in a Newman projection, the double bond bisects one of the R-C-R angles, is called a 'bisecting conformation'. The other conformation, in which X is synperiplanar to one of the R group, is called an 'eclipsing conformation'.



Projections for $CH_3\text{-}CH_2\text{-}CHO$

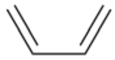
bisecting conformation

eclipsing conformation

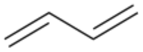
P-94.3.1.3 Stereodescriptors s-*cis* and s-*trans*

The spatial arrangement of two conjugated double bonds about the intervening single bond is described as 's-*cis*' if 'synperiplanar' and 's-*trans*' if 'antiperiplanar'. This descriptor should not be applied to other systems such as *N*-alkyl amides (use '*E/Z*' or '*sp/ap*').

Examples:



s-*cis*



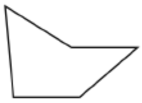
s-*trans*

P-94.3.2 Stereodescriptors for denoting the conformations of alicyclic rings

P-94.3.2.1 Envelope conformation

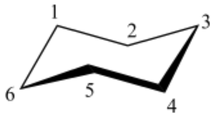
The envelope conformation is the conformation of a five-membered ring in which four atoms are coplanar and one atom projects out of the plane.

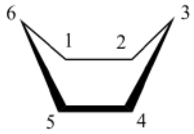
Example:

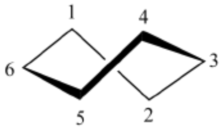


P-94.3.2.2 Chair, boat, and twist conformations

When carbon atoms 1, 2, 4, and 5 of a six-membered ring occupy coplanar positions and when carbon atoms 3 and 6 are on opposite sides of the plane the conformation is called a chair form. It is a boat form when carbon atoms 3 and 6 are on the same side of the plane. The conformation passed through in the interconversion of two boat forms of six-membered ring is called the twist form; this term is preferred to skew boat, skew form, or stretched form.



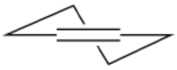




In carbohydrate stereochemistry, the term twist refers to a five-membered ring and the twist conformation is referred to as skew.

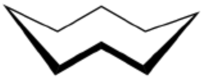
P-94.3.2.3 Half-chair

A molecule of a monounsaturated six-membered ring is described as being in a ‘half-chair’ conformation according as the atoms not directly linked to the double bond lie on opposite sides of the plane.

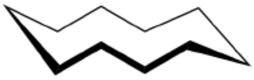


P-94.3.2.4 Crown conformation

The conformation of a saturated cyclic molecular entity, containing an even number (≥ 8) of atoms in the ring, in which these atoms lie alternately in each of two parallel planes and are symmetrically equivalent (D_{4d} for cyclooctane, D_{5d} for cyclodecane, etc.), is called a ‘crown conformation’.



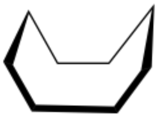
cyclooctane



cyclodecane

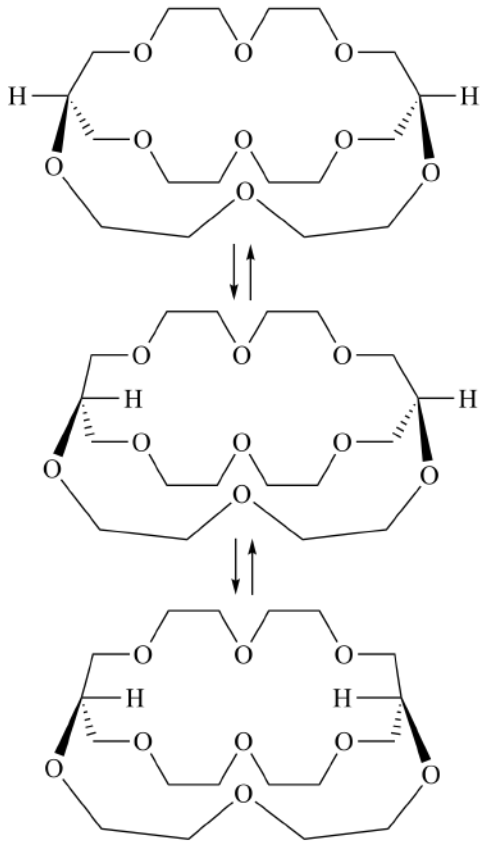
P-94.3.2.5 Tub conformation

The conformation of an eight-membered ring in which the four atoms forming one pair of diametrically opposite bonds in the ring lie in one plane and all other ring atoms lie on one side of that plane is called a ‘tub conformation’.

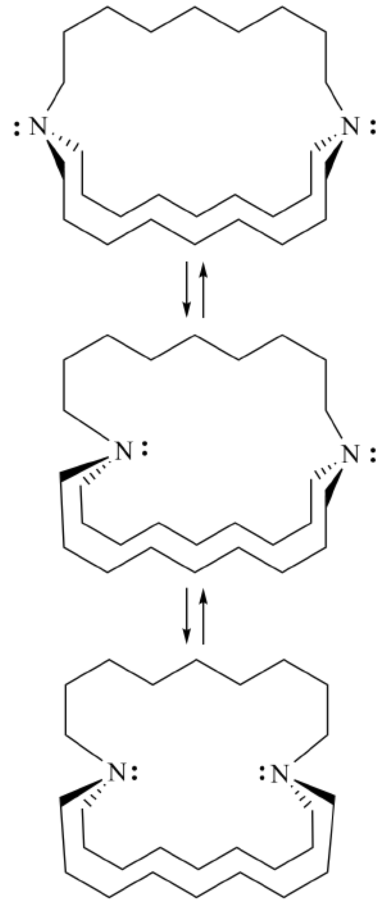


P-94.3.2.6 In-out isomerism
In-out isomerism is found in bicyclic systems having bridges long enough to allow the bridgehead exocyclic bond or lone pair of electrons to point either inside the structure or outside.

Example 1:



Example 2:



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Chapter P-10 PARENT STRUCTURES FOR NATURAL PRODUCTS AND RELATED COMPOUNDS

P-100 Introduction
P-101 Nomenclature for natural products based on parent hydrides (alkaloids, steroids, terpenes, carotenes, corrinoids, tetrapyrroles, and similar compounds)
P-102 Carbohydrate nomenclature
P-103 Amino acids and peptides
P-104 Cyclitols
P-105 Nucleosides
P-106 Nucleotides
P-107 Lipids

P-100 INTRODUCTION

In the field of natural products, three levels of nomenclature are recognized. A new compound, isolated from a natural source, is generally given a ‘trivial’ name. By common usage, these trivial names are commonly related to the biological origin of the material, but frequently not in a rational way, since the available structure is not known with great detail. These trivial names are considered to be ephemeral and replaced for chemical purposes by names describing the skeleton, the characteristic groups, and the organyl substituent groups.

When the full structure is known, a ‘systematic name’ may be generated in accordance with Rules described in Chapters P-1 through P-9 of these recommendations. However, this name may be too cumbersome to be continually inserted into the text of a scientific paper. To overcome this difficulty and show the close similarity to related compounds, a ‘semisystematic name’ can be formed. Preferred IUPAC names (PINs) are not identified for the compounds in this Chapter. The choice between a semisystematic name and a systematic name will be made in cooperation with the IUPAC-IUBMB Joint Commission on Biochemical Nomenclature and will appear in a future publication.

Semisystematic names are based on specific parent structures, generally including the configuration, that can later on be used to describe a compound fully by using the rules of systematic nomenclature. There are two general types of semisystematic parent structures used for naming natural products and related compounds:

(a) parent hydrides, i.e., structures that do not have terminal heteroatoms or functional groups and therefore consist only of skeletal atoms and hydrogen, for example, in steroid (ref.16), terpene, carotene (ref. 40), corrinoid (ref. 45), tetrapyrrole (ref. 17), lignan and neolignan (ref. 46), and alkaloid nomenclature. This type of semisystematic parent is analogous to the parents described in Chapter P-2 and is treated in the same manner to generate complete names;

(b) functional parents, which are analogous to the functional parents described in Section P-34, and used in amino acid and peptide (ref. 18), carbohydrate (ref. 27), cyclitol (ref. 39), nucleoside and nucleotide (ref. 47), and lipid (ref. 48) nomenclature; they have characteristic groups implied in their name, and can be modified by specific rules and by methods used in systematic nomenclature.

Section P-101 describes the rules to form trivial names and semisystematic names used as parent hydrides, and those related to their skeletal transformation and functionalization for naming alkaloids, steroids, terpenes, and some related compounds. Section P-102 describes the rules for naming carbohydrates, P-103 deals with the nomenclature of amino acids and peptides, P-104 describes the nomenclature for cyclitols, P-105 and P-106 deal with nucleosides and nucleotides, and finally P-107 discusses the nomenclature of lipids. If difficulties are encountered, consultation of the full publications may be necessary, as indicated in each Section.

P-101 NOMENCLATURE FOR NATURAL PRODUCTS BASED ON PARENT HYDRIDES, (ALKALOIDS, STEROIDS, TERPENES, CAROTENES, CORRINOIDS, TETRAPYRROLES, AND SIMILAR COMPOUNDS)

This Section is based on the recent publication ‘Revised Section F: Natural Products and Related Compounds, IUPAC Recommendations 1999’ and the additional document ‘Corrections and Modifications 2004’ (ref. 9).

P-101.1 Biologically based trivial names
P-101.2 Semisystematic nomenclature for natural products (stereoparent hydrides)
P-101.3 Skeletal modifications of parent structures
P-101.4 Replacement of skeletal atoms
P-101.5 Addition of rings and ring systems
P-101.6 Modification of the degree of hydrogenation of parent structures
P-101.7 Derivatives of parent structures
P-101.8 Further aspects of configurational specification

P-101.1 BIOLOGICALLY BASED TRIVIAL NAMES

P-101.1.1 When a compound is isolated from a natural source and a trivial name is required, the name should be based, whenever possible, on the family, genus, or species name of the biological material from which it has been isolated. If appropriate, the class or order might also be used for the name of a compound that occurs in a number of related families.

P-101.1.2 The ending 'une' or, for euphonic reasons, 'iune' is used to indicate that the trivial name it terminates describes a compound of unknown structure.

P-101.2 SEMISYSTEMATIC NOMENCLATURE FOR NATURAL PRODUCTS (stereoparent hydrides)

P-101.2.0 Introduction
P-101.2.1 General guidelines for choosing a parent structure
P-101.2.2 Structural features allowed for parent structures
P-101.2.3 Numbering of parent structures
P-101.2.4 Identification of individual rings
P-101.2.5 Atomic connector, terminal segment and bond connector
P-101.2.6 Stereochemical configuration of parent structures
P-101.2.7 Semisystematic names of recommended fundamental parent structures

P-101.2.0 Introduction

Many naturally occurring compounds belong to well defined structural classes, each of which can be characterized by a set of parent structures that are closely related structurally, that is, each can be derived from a fundamental parent structure by one or more defined operations used in systematic substitutive nomenclature (see P-13).

As soon as the structure of a simple new natural product has been fully determined, the trivial name should be abandoned in favor of a systematic name formed by the Rules prescribed in Chapters P-1 through P-9 for systematic nomenclature of organic compounds. For a more complicated structure, an existing semisystematic name listed in P-101.2.7 is used to fully name the compound. If a previously known parent structure cannot be found, a new parent structure is formed and numbered as follows. To form and number a new parent structure, the procedure described in the following subsections is followed.

P-101.2.1 General guidelines for choosing a parent structure

P-101.2.1.1 A fundamental parent structure should reflect the basic skeleton (including nonterminal heteroatoms and hetero groups) that is common to most compounds of the class.

P-101.2.1.2 Fundamental parent structures should be chosen so that as many natural products as possible can be derived from each by well defined operations and rules of the nomenclature of organic compounds.

P-101.2.1.3 A fundamental parent structure should include as much configuration as possible that is common to the relevant class of natural products. Such parent structures are called 'stereoparents'.

P-101.2.2 Structural features allowed for parent structures

The following rules are applicable to new parent structures. Existing parent structure names are considered as retained names if they do not follow the new rules (see Table 10.1).

P-101.2.2.1 A fundamental parent structure should exceptionally include rings that are part of a characteristic group, such as a lactone or cyclic acetal.

P-101.2.2.2 A fundamental parent structure should not contain terminal heteroatoms or characteristic groups (see P-101.2.1.1).

P-101.2.2.3 A fundamental parent structure should contain acyclic hydrocarbon groups that occur in most of the compounds in the natural product class.

P-101.2.2.4 A fundamental parent structure should be as nearly fully saturated or fully unsaturated in terms of maximum number of noncumulative double bonds (mancude rings), while still representing the level of saturation (or unsaturation) of as many related compounds as possible.

P-101.2.2.5 A semisystematic name for a fundamental parent structure should be derived, as far as possible, from a trivial name formed in accordance with P-101. The endings to be used in place of 'une' or 'iune' must be assigned as follows:

(a) 'ane', if the entire stereoparent hydride is fully saturated;

(b) 'ene', if the cyclic or the main chain of the acyclic part contains the maximum number of noncumulative double bonds;

(c) 'arane', if, in an otherwise fully saturated parent structure, one or more individual mancude rings is present.

Existing names of parent structures in which endings are different from those indicated above, for example morphinan and ibogamine, are exceptions and treated as retained names.

P-101.2.2.6 Indicated hydrogen, as defined in P-14.7, P-25.7 and P-58.2, is used to describe isomers of fundamental parent structures.

P-101.2.3 Numbering of parent structures

P-101.2.3.1 A numbering pattern established among a group of structurally related natural products is used for numbering the skeletal atoms of the fundamental parent structure, providing that all skeletal atoms have been included in the numbering system.

P-101.2.3.2 If no numbering pattern has been become established among the members of a group of structurally related natural products, the fundamental parent structure is numbered according to the following guidelines:

(a) examine the skeleton to identify the senior ring or ring system, according to P-44. The locant '1' is assigned to the atom of the senior ring system whose locant would be '1' according to systematic numbering for that particular ring or ring system;

(b) assign all skeletal atoms of the senior ring system consecutive Arabic numbers, including atoms of fusion positions in fused ring systems, beginning with the locant '1', and following the path prescribed for that particular type of ring or ring system;

(c) number acyclic substituents to skeletal atoms of ring components or connecting acyclic structures each in its entirety, including branches, in order of the increasing value of the locant of the skeletal atom to which it is attached;

(d) number skeletal atoms of acyclic connections to other ring or ring systems, if any, consecutively beginning with the atom next to the senior ring system, followed by the skeletal atoms of the other rings or ring systems as prescribed in (b) above; if two or more acyclic connections to other rings or ring systems are present, the one attached to the senior ring or ring system at the lowest numbered position is numbered first, then the ring attached to it, followed by the acyclic connector at the next lower position of the senior ring or ring system, etc.;

(e) number the larger group, in terms of the number of skeletal atoms, between two groups at a geminal disubstituted position first; if there is still a choice, alphanumerical order is followed (Rule P-14.5). If the two groups are then identical and attached to a stereoparent structure properly drawn (see Appendix 3), the group that is stereochemically 'α' (according to P-101.2.6) is numbered first; if the two groups are identical and attached to an acyclic terminal double bond, the group '*trans*' to the main chain is numbered first, as described in the carotenoid recommendations (Rule 12.4 in ref. 40).

P-101.2.4 Identification of individual rings

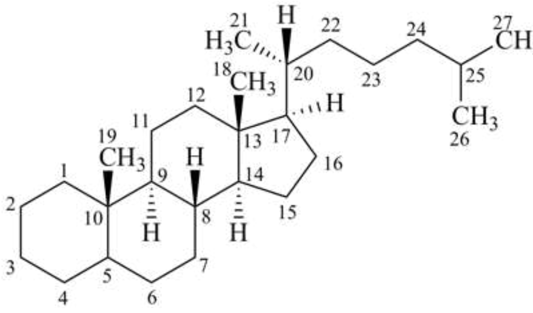
Since locants are used to describe skeletal modifications, as indicated in P-101.3, the identification of individual rings by letters A, B, C, etc., used in the past is no longer recommended, except for the rather special case of the removal of a terminal ring (see P-101.3.6). Nevertheless, to provide continuity with the use of this system, names using letters to identify rings are given where appropriate, but are no longer recommended.

P-101.2.5 Atomic connector, terminal segment, and bond connector

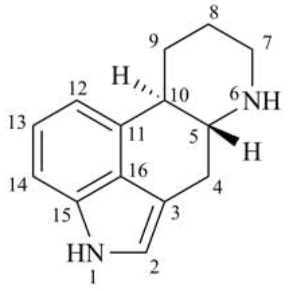
For nomenclature purposes, the fundamental parent structures are described by specific arrangements of atoms or groups of atoms called 'atomic connectors', 'terminal segments' and 'bond connectors', that must be taken into consideration in accordance with the additive or subtractive operations modifying a fundamental parent structure.

An 'atomic connector' is a chain of homogeneous skeletal atoms of the same element connecting any combination of bridgehead or ring junction atoms, rings, or ring systems (i.e. ring assemblies), substituted skeletal atoms in parent structure, or heteroatoms. A ‘terminal segment’ of a skeletal structure is an acyclic portion of homogeneous skeletal atoms connected at only one end by the features of structure that terminate atomic connectors. A ‘bond connector’ is a connection between any combination of bridgehead or ring junction atoms, rings, or ring systems (i.e. ring assemblies), substituted skeletal atoms, or heteroatoms. The structures below illustrate atomic connectors, bond connectors, and terminal segments. The use of these terms is further illustrated in P-101.3.1 in relation to the removal of skeletal atoms denoted by the prefix ‘nor’.

Examples:



cholestane



ergoline

atomic connectors:
in cholestane: 1-4, 6-7, 11-12, 15-16, and 22-24
in ergoline: 2, 4, 7-9, and 12-14

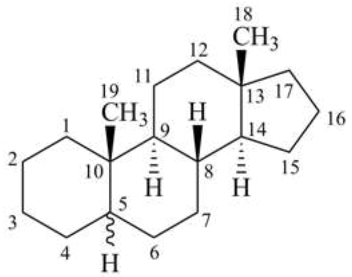
terminal portions:
in cholestane: 18, 19, 21, 26, and 27
in ergoline: none

bond connectors:
In cholestane: 5-10, 8-9, 8-14, 9-10, 13-14, 13-17, and 17-20
In ergoline: 1-15, 3-16, 5-6, 5-10, 10-11, 11-16, and 15-16

P-101.2.6 Stereochemical configuration of parent structures

The name of a fundamental parent structure usually implies the absolute configuration of all chirality centers and the configuration of double bonds, when applicable, without further specification. All chirality must be defined so that for example with a steroid the stereochemistry at ‘C-5’, when relevant, is indicated by α, β or ξ. When a planar or quasi planar system of rings is denoted as a projection, as in this recommendation, an atom or group attached to the ring is called ‘α’ if it lies below or ‘β’ if it lies above the plane of the paper. Use of this system requires the orientations of structure as given in the examples used to exemplify the various rules and in Appendix 3. In the example below, the implied configurations shown define the attached hydrogen atoms and methyl groups at positions ‘8’, ‘10’, and ‘13’ as ‘β’, and at positions ‘9’ and ‘14’ as ‘α’; here, the configuration of the hydrogen atom at position 5 is not known and thus the orientation is ‘ξ’ (xi), denoted by a wavy line in the formula. The stereodescriptors ‘α’, ‘β’, and ‘ξ’ used to describe implicit or indicated configuration are cited before the name of the fundamental parent structure without parentheses.

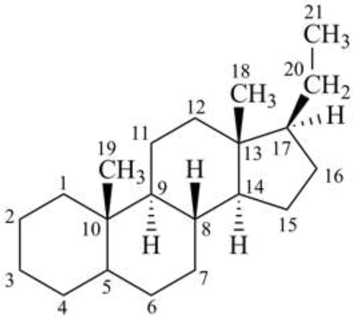
The ‘α/β’ symbolism is used as defined above and extended in the following way to express different aspects of the configuration of modified fundamental parent structures.

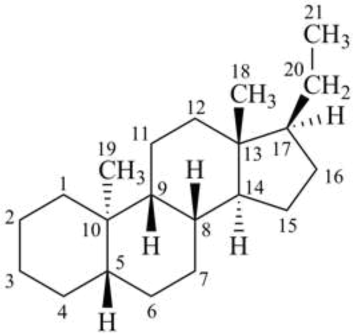


P-101.2.6.1 Configurations that are different from those in the parent structure

P-101.2.6.1.1 At chirality centers, the ‘α/β’ system is used as described in IUPAC- IUBMB recommendations for the nomenclature of steroids (ref. 16). Each chirality center is described by the stereodescriptor ‘α’, ‘β’, or ‘ξ’ to indicate a configuration that must be specified and those that are inverted. The symbols ‘α’, ‘β’, or ‘ξ’, preceded by the appropriate locants, are placed immediately at the beginning of the name of the fundamental parent structure. In the following examples, configuration at ‘C-5’ must be specified; configurations at bridgeheads ‘C-9’ and ‘C-10’ are inverted when compared with those of the fundamental parent structure. This method is preferred to the alternatives described in P-101.2.6.1.2.

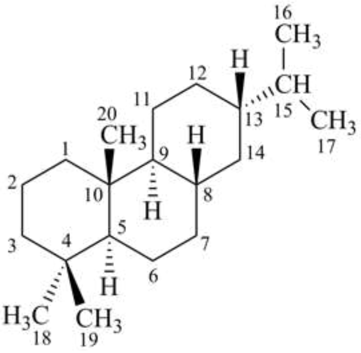
Example:

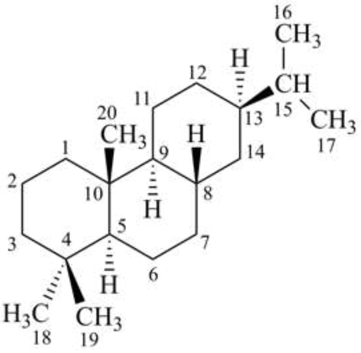

pregnane
(fundamental parent structure)


5β,9β,10α-pregnane

A change in configuration of a nonbridgeheaded side chain that is part of the parent is denoted by the method specified for 'C-17' of steroids (see 3S-5.2, ref. 16), where 'α' or 'β' refers to the side chain itself and not to the hydrogen atom in the same position.

Example:

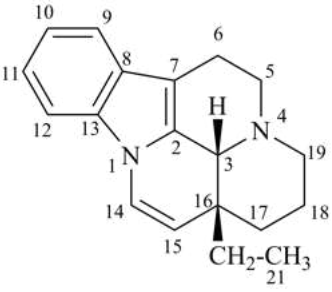

abietane
(fundamental parent structure)


13β-abietane

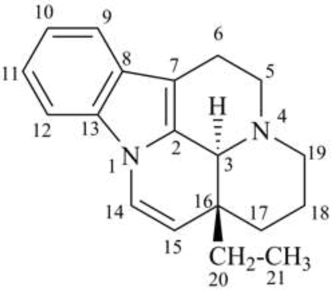
P-101.2.6.1.2 Configurational inversion at one of stereogenic centers whose configuration is implied or stated in the name of the fundamental parent structure can be indicated by the italicized prefix '*epi*' (derived from 'epimer') placed at the front of the name of the parent structure and prefixed by the locant of the affected atom.

The name 13β-abietane, described above in P-101.2.6.1.1, can also be named 13-*epi*-abietane.

Example:



eburnamenine
(fundamental parent structure)



3-*epi*-eburnamenine
3α-eburnamenine

P-101.2.6.1.3 The stereodescriptors ‘*R*’ and ‘*S*’

The stereodescriptors ‘*R*’ and ‘*S*’ are used to describe the absolute configuration not specified by the ‘α/β’ system described above, in accord with the CIP priority system and the rules and conventions described in Chapter 9. The stereodescriptors ‘*R*’ and ‘*S*’ are also used when a ring is opened and two chirality centers are created, one of which may rotate, as described for vitamin D in P-101.8.4.

P-101.2.7 Semisystematic names of recommended parent structures are listed in Table 10.1. Structures are shown in Appendix 3.

Table 10.1 Names of fundamental stereoparent structures (nonlimiting)

(a) **alkaloids**

aconitane
ajmalan
akuammilan
alstophyllan
aporphine
aspidofractinine
aspidospermidine
atidane
atisine
berbaman
berbine
cephalotaxine
cevane
chelidonine
cinchonan
conanine
corynan
corynoxan
crinan
curan
daphnane
dendrobane
eburnamenine
emetan
ergoline
ergotaman
erythrinan
evonimine
evonine
formosanan
galanthamine
galanthan
hasubanan
hetisan
ibogamine
kopsan
lunarine
lycopodane
lycorenan
lythran
lythranidine
matridine
morphinan
nupharidine
ormosanine
18-oxayohimban
oxyacanthan
pancracine
rheadan
rodiasine
samandarine
sarpagan
senecionan
solanidane
sparteine
spirosolane
strychnidine
tazettine
tropane
tubocuraran
tubulosan
veratraman
vincaleukoblastine
vincane
vobasan
vobtusine
yohimban

(b) **steroids**

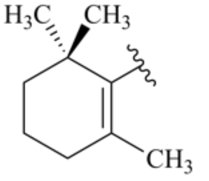
androstane
cholestane
gorgostane

bufanolide
campestane
cardanolide
cholane
ergostane
estrane
furostan
gonane
poriferastane
pregnane
spirostan
stigmastane

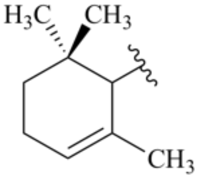
(c) **terpenes** (all are parent hydrides except retinal)

abietane
ambrosane
aristolane
atisane
beyerane
bisabolane
bornane
cadinane
carane
β,φ-carotene*
β,ψ-carotene*
ε,κ-carotene*
ε,χ-carotene*
caryophyllane
cedrane
dammarane
drimane
eremophilane
eudesmane
fenchane
gammacerane
germacrane
gibbane
grayanotoxane
guaiane
himachalane
hopane
humulane
kaurane
labdane
lanostane
lupane
menthane (*p*-isomer)
oleanane
ophiobolane
picrasane
pimarane
pinane
podocarpane
protostane
retinal
rosane
taxane
thujane
trichothecane
ursane

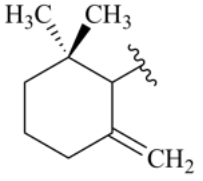
* Four different carotenes are exemplified; there are 28 carotene parent structures derived from all permutations of the seven following end groups:



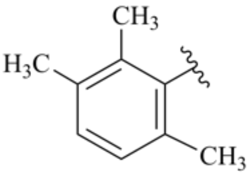
β (beta)



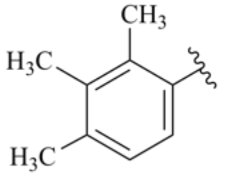
ε (epsilon)



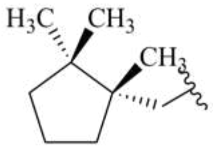
γ (gamma)



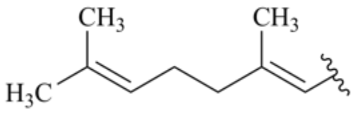
φ (phi)



χ (chi)



κ (kappa)



ψ (psi)

(d) **Miscellanous** (all are parent hydrides except cepham and penam)

21*H*-biline
cepham
corrin
flavan
isoflavan
lignane
neoflavan
neolignane
penam
porphyrin
prostane
thromboxane

P-101.3 SKELETAL MODIFICATIONS OF PARENT STRUCTURES

P-101.3.0 Introduction
P-101.3.1 Removal of skeletal atoms without affecting the number of rings
P-101.3.2 Addition of skeletal atoms without affecting the number of rings
P-101.3.3 Bond formation

P-101.3.4 Bond cleavage
P-101.3.5 Bond migration
P-101.3.6 Removal of a terminal ring
P-101.3.7 Combination of the prefixes ‘cyclo’, ‘seco’, ‘apo’, ‘homo’, and ‘nor’

P-101.3.0 Introduction

The skeleton of parent structures can be modified in many ways, contracted, expanded, or rearranged by using operations described in P-13. These operations are denoted by specific nondetachable prefixes that are added to the name of the parent structure. Changes affecting the configuration must be shown as indicated in P-101.2.6. In natural product nomenclature, the number of operations is not subject to limitations.

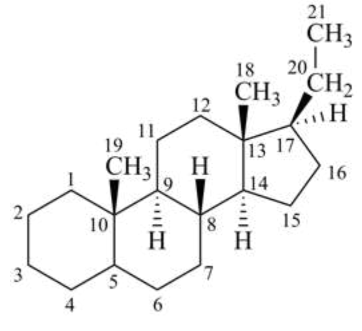
This Section supersedes the Section F Rules (ref. 9) and Rules A-71 through A-75 related to terpene hydrocarbons as prescribed in the 1979 Recommendations (ref. 1).

P-101.3.1 Removal of skeletal atoms without affecting the number of rings

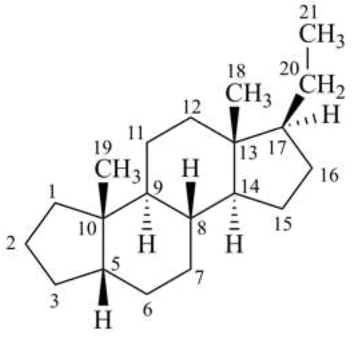
P-101.3.1.1 The removal of an unsubstituted skeletal atom, saturated or unsaturated, from a ring or of an unsubstituted skeletal atom from a saturated acyclic portion of a fundamental parent structure with its attached hydrogen atom(s) is described by the nondetachable prefix ‘nor’; the loss of two or more such skeletal atoms is indicated by the usual numerical multiplicative prefixes ‘di’, ‘tri’, etc. added before ‘nor’.

The position of the skeletal atom that is removed is denoted in all cases by its locants in the numbering of the fundamental parent structure. Although, because the locant of each skeletal atom removed is cited, an unambiguous name can be generated by the removal of any skeletal atom, carbon atom or heteroatom, it is traditional to remove skeletal atoms with the highest possible locant in an atomic connector in a cyclic portion of the skeletal structure. In carotenoids, as an exception, the locant attached to ‘nor’ is the lowest possible (see Rule Carotenoid 5.1, ref. 40).

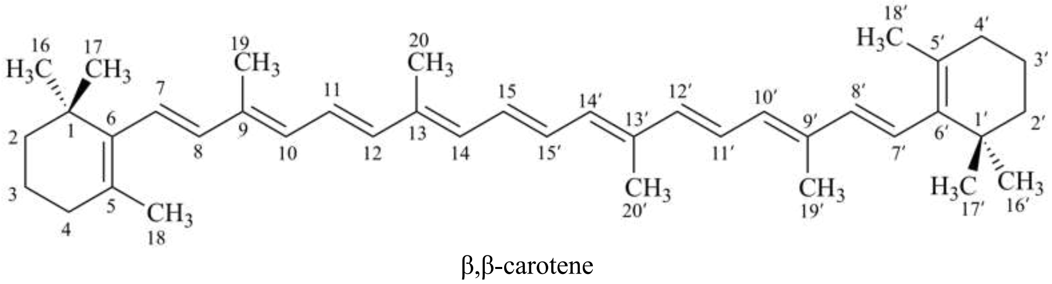
Examples:



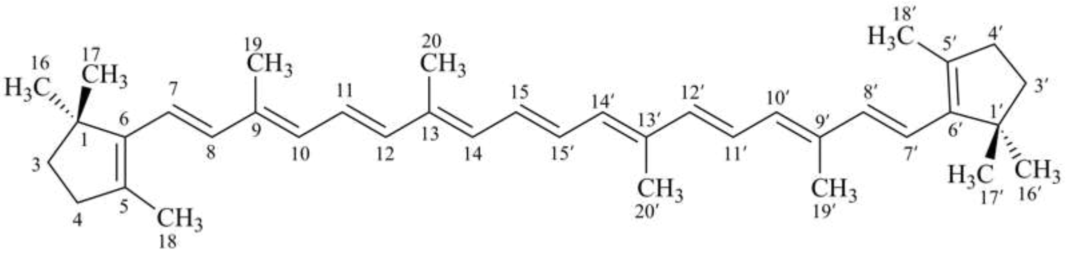
pregnane
(fundamental parent structure)



4-nor-5β-pregnane



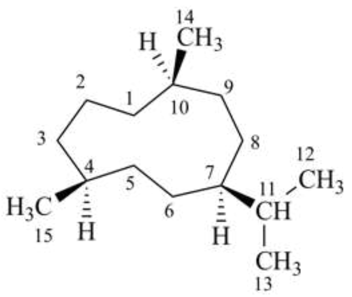
β,β-carotene
(fundamental parent structure)



2,2′-dinor-β,β-carotene

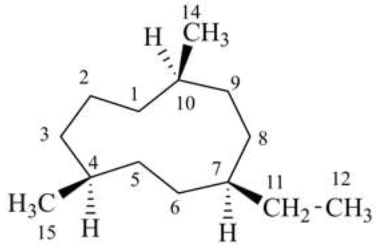
In an acyclic portion of a skeletal structure, the skeletal atom removed preferably is the one of an acyclic atomic connector or a terminal segment nearest to the free end of this acyclic portion (this is done in order to maintain as far as possible the numbering of structural features of the compound and of compounds derived from it).

Examples:



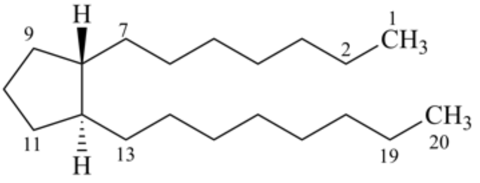
14
H
CH3
1
2
3
4
5
6
7
8
9
10
11
12
CH3
CH
H3C
15
H
H
CH3
13

germacrane
(fundamental parent structure)



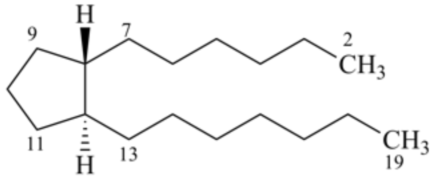
14
H
CH3
1
2
3
4
5
6
7
8
9
10
11
12
H3C
15
H
H
CH2-CH3

13-norgermacrane
(1*R*,4*s*,7*S*)-4-ethyl-1,7-dimethylcyclodecane
(position 1 is position 10 for germacrane)



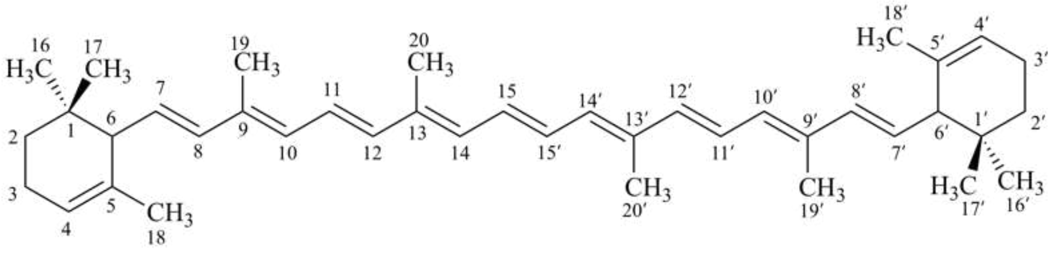
H
9
7
1
2
CH3
CH3
11
H
13
19
20

prostane
(fundamental parent structure)



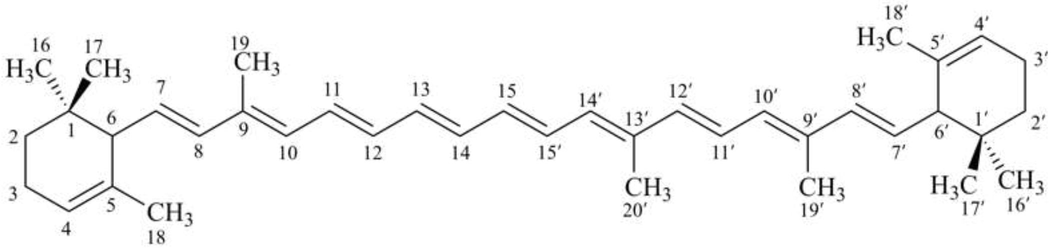
H
9
7
2
CH3
CH3
11
H
13
19

1,20-dinorprostane
(1*S*,2*S*)-1-heptyl-2-hexylcyclopentane



16
17
H3C
CH3
19
CH3
20
CH3
18′
H3C
1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
15′
14′
13′
12′
11′
10′
9′
8′
7′
6′
5′
4′
3′
2′
1′
CH3
18
CH3
20′
CH3
19′
H3C
17′
CH3
16′

ε,ε-carotene
(fundamental parent structure)

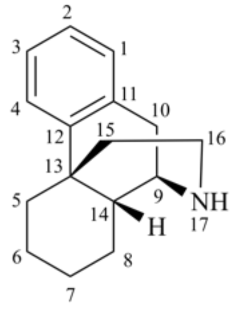


16
17
H3C
CH3
19
CH3
18′
H3C
1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
15′
14′
13′
12′
11′
10′
9′
8′
7′
6′
5′
4′
3′
2′
1′
CH3
18
CH3
20′
CH3
19′
H3C
17′
CH3
16′

20-nor-ε,ε-carotene
(see P-14.3.5 for use of unprimed and primed locants)

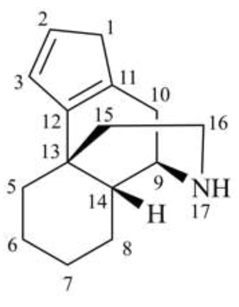
P-101.3.1.2 When the removal of an unsaturated skeletal atom from a mancude ring (containing the maximum number of noncumulative double bonds) in the fundamental parent structure results in the creation of a saturated ring position, this position is described by indicated hydrogen (see P-14.7). In names, the symbol *H*, denoted by the appropriate locant, is cited at the beginning of the name modified by the nondetachable prefix.

Example:



1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
NH
17
H

morphinan
(fundamental parent structure)



1
2
3
5
6
7
8
9
10
11
12
13
14
15
16
NH
17
H

1*H*-4-normorphinan

P-101.3.2 Addition of skeletal atoms without affecting the number of rings

P-101.3.2.1 The addition of a methylene (–CH_2–) group between two skeletal atoms of a fundamental parent structure is described by the nondetachable prefix 'homo'; the addition of two or more methylene groups is indicated by the numerical multiplicative prefixes 'di', 'tri', etc. Positions of the inserted methylene groups in the modified fundamental parent structure are indicated by the locants of the added methylene groups cited in front of the prefix 'homo', preceded by multiplicative prefixes when required.

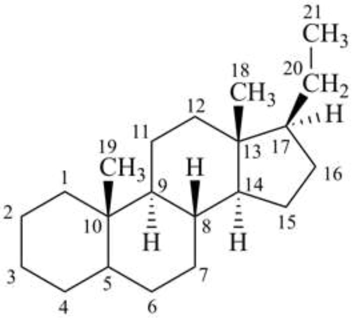
The assignment of the locants to an added methylene group depends on whether it is considered to be inserted into an atomic connector or terminal acyclic portion or into a bond connector.

P-101.3.2.2 Numbering of additional skeletal atoms

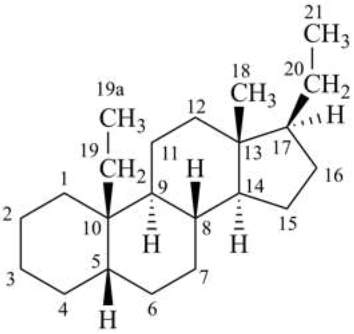
P-101.3.2.2.1 Methylene groups inserted into an atomic connector or into a terminal segment are identified by adding a letter 'a', 'b', etc., to the locant of the highest numbered skeletal atom of the atomic connector or terminal portion consistent with the location of double bonds remaining in the structure. If there are equivalent atomic connectors, the highest atomic connector is chosen, and the methylene group is inserted after the highest numbered skeletal atom in that connector.

Addition of acyclic side chains or extension of terminal portions of a side chain already attached to the stereoparent hydride may also be done by principles of substitutive nomenclature. The added substituent(s) are numbered as described above for 'homo' atoms.

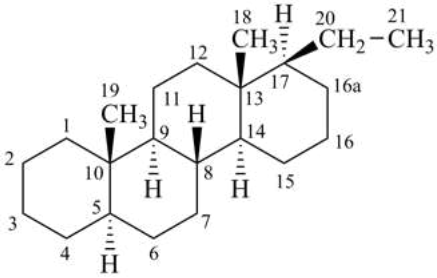
Examples:



pregnane
(fundamental parent structure)



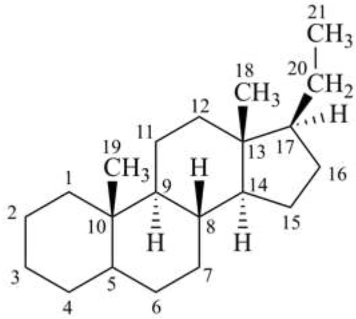
19a-homo-5β-pregnane
(not 19-methyl-5β-pregnane;
alkyl substitution of a side chain is not allowed)



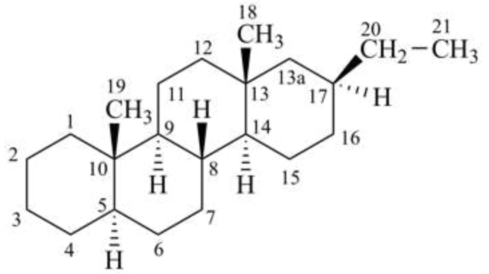
16a-homo-5α-pregnane

P-101.3.2.2.2 Methylene groups inserted into a bond connector are identified by citing both locants of the skeletal atoms terminating the bond connector enclosing the second (higher) number in parentheses, followed by a letter 'a', 'b', etc. according to the number of methylene groups

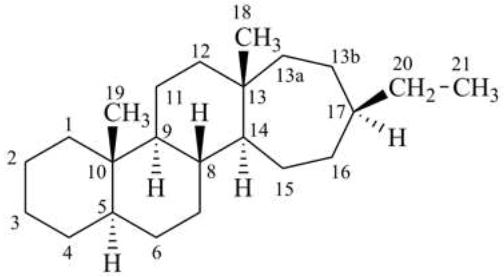
Examples:


21
CH_3
20
CH_2
18
CH_3
H
12
11
13
17
19
CH_3
H
16
1
9
14
2
10
8
15
H
H
3
5
7
4
6

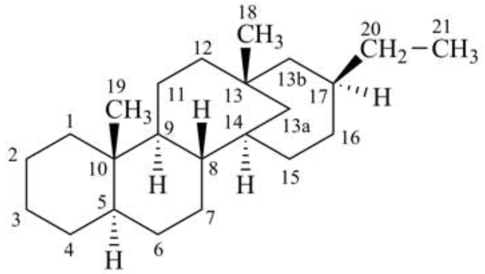
pregnane
(fundamental parent structure)


18
CH_3
20
21
CH_2-CH_3
12
13a
19
11
13
17
H
CH_3
H
1
9
14
16
2
10
8
15
H
H
3
5
7
4
6
H

13(17)a-homo-5α-pregnane


18
CH_3
12
13b
20
21
13a
CH_2-CH_3
19
11
13
17
CH_3
H
H
1
9
14
2
10
8
16
H
H
15
3
5
4
6
H

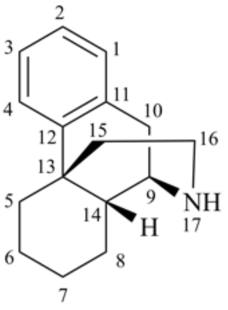
13(17)a,13(17)b-dihomo-5α-pregnane
[this has been called
D(17a,17b)dihomo-5α-pregnane;
see Rule 2S-7.3, ref. 16]


18
CH_3
20
21
CH_2-CH_3
12
13b
19
11
13
17
H
CH_3
H
14
13a
1
9
16
2
10
8
15
H
H
3
5
7
4
6
H

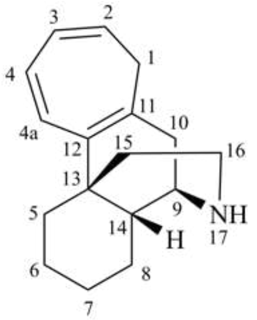
13(14)a,13(17)b-dihomo-5α-pregnane

P-101.3.2.2.3 The insertion of a methylene group into a mancude ring or ring system (that contains the maximum number of noncumulative double bonds) or into a system of conjugated double bonds may create a saturated ring position that is described by 'indicated hydrogen' (see P-14.7 and P-58.2). The position of the methylene group is prescribed by P-101.3.2.2.2, even though the saturated ring position may be elsewhere in the unsaturated ring system as denoted by the appropriate locant for the indicated hydrogen; this is a change for names of the homoporphyrins (see ref. 17, Rule TP-5.1). Two tautomeric forms, (**A**) and (**B**), are represented below and specifically numbered and named.

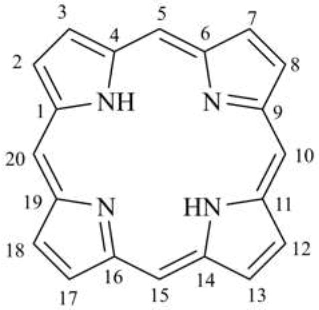
Examples:



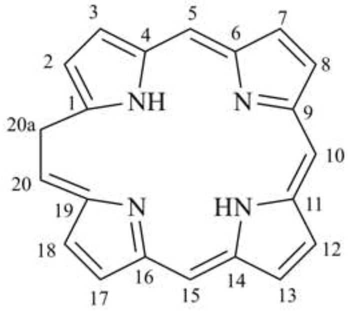
morphinan
(fundamental parent structure)



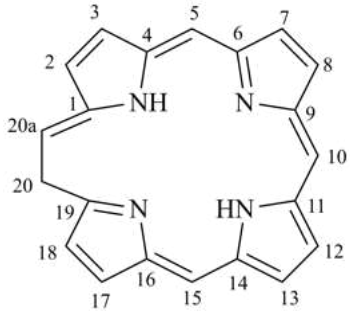
1*H*-4a-homomorphinan



porphyrin
(fundamental parent structure)



(**A**) 20a*H*-20a-homoporphyrin



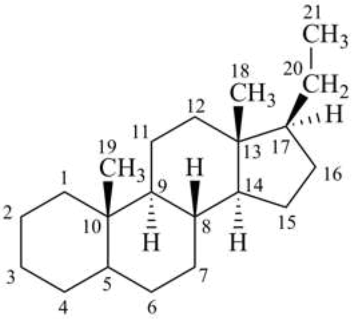
(**B**) 20*H*-20a-homoporphyrin

P-101.3.3 Bond formation

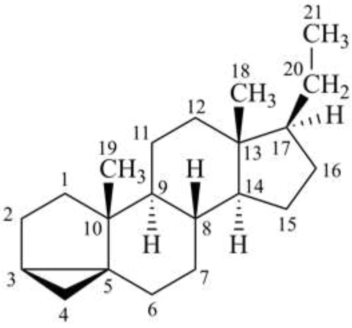
The creation of an additional ring by a conjunctive operation (see P-13.5.3) by means of a direct link between any two atoms of a parent structure is described by the nondetachable prefix 'cyclo' (not italicized) preceded by the locants of the skeletal atoms so connected. When necessary, the configuration created by the new bond is denoted by α, β, or ξ descriptors in accord with P-101.2.6, or by describing the configuration of the hydrogen atom in accordance with P-101.2.6.1.3.

Configurations of the fundamental parent structure are retained. New configurations of the ring atoms having one hydrogen atom still present are indicated by the 'α/β' stereodescriptors as described in P-101.2.6, or, if necessary, by the sequence rule method (*R*/*S*). The projection of the hydrogen atom below, 'α', or above, 'β', the plane of the ring system is indicated by the appropriate symbol and a capital italic letter *H* following the locant of the ring atom in the structure, all enclosed in parentheses, and cited before the appropriate prefix, in this case 'cyclo' (see P-101.3.5.1 for the prefix 'abeo'). This method of citation differs from that used in the Steroid Rules (Rule 3S-7.5, ref. 16).

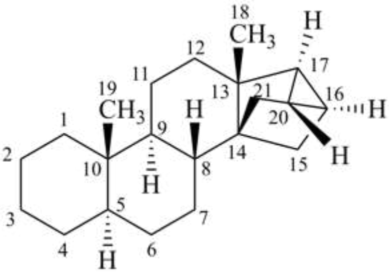
Examples:



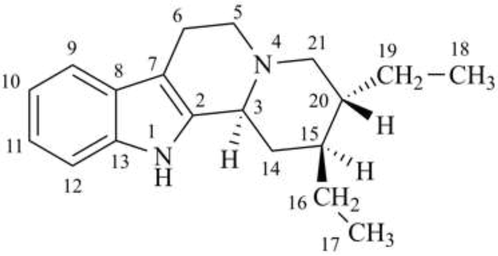
pregnane
(fundamental parent structure)



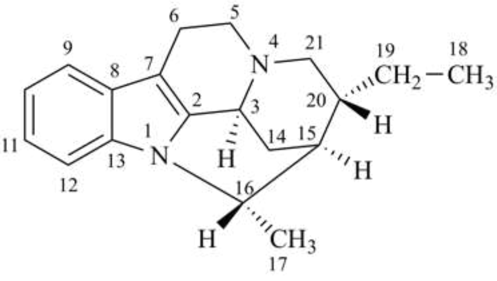
3α,5-cyclo-5α-pregnane



(20*S*)-14,21:16β,20-dicyclo-5α,14β-pregnane



corynan
(fundamental parent structure)

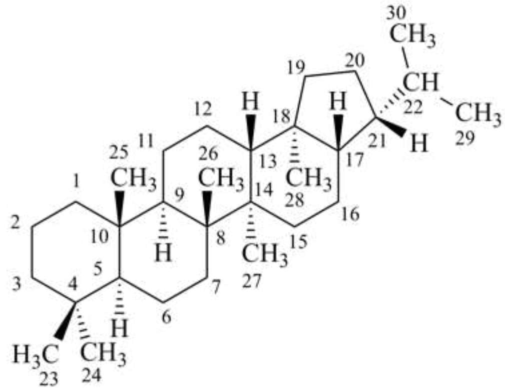


(16β*H*)-1,16-cyclocorynan

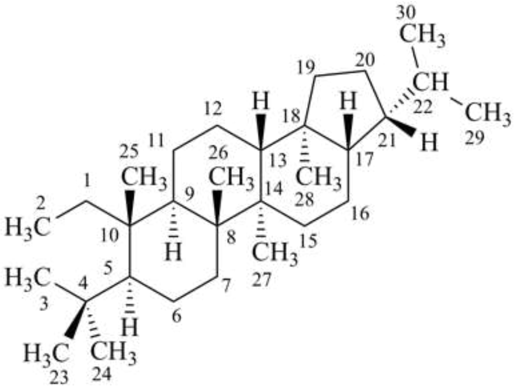
P-101.3.4 Bond cleavage

P-101.3.4.1 Cleavage of a ring bond (saturated or unsaturated) with the addition of the appropriate number of hydrogen atoms at each new terminal group thus created is indicated by the prefix ‘seco’ (not italicized) and the locants of the cleaved bond. The original numbering is retained.

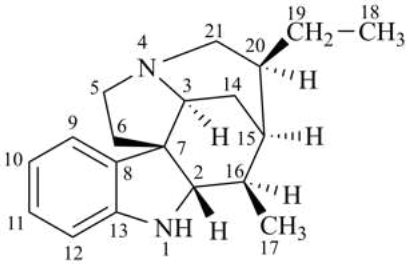
Examples:



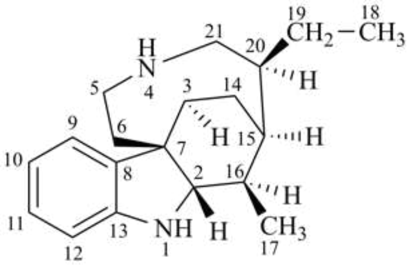
hopane
(fundamental parent structure)



2,3-secohopane



curan
(fundamental parent structure)



3,4-secocuran

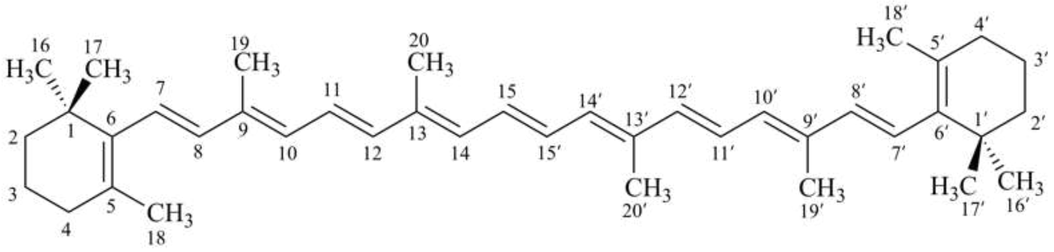
P-101.3.4.2 The prefix 'apo'

The unitalicized prefix 'apo' preceded by a locant is used to indicate removal of all of a side chain of a fundamental parent structure beyond the skeletal atom corresponding to that locant. Removal of two or more side chains is indicated by the prefixes 'diapo', 'triapo', etc., preceded by the required locants. Numbering of the skeletal atoms of the fundamental parent structure is retained in the resulting fragment.

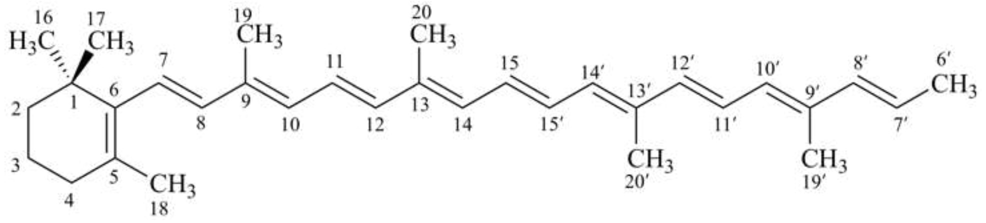
The following procedure is used only in carotenoid nomenclature (see ref. 40, Rule Carotenoid 10). The unitalicized prefix 'apo', preceded by a locant, is used to indicate that all of the molecule beyond the carbon atom corresponding to that locant has been replaced by a hydrogen atom. A side-chain methyl group is not considered to be 'beyond' the carbon atom to which it is attached. Removal of fragments from both ends of a molecule is indicated by using the numerical multiplying prefixe 'di', preceded by two locants. Numbering of the skeletal atoms in the parent structure is retained in the resulting fragment.

The prefix and its locant immediately precede the parent name unless the locant associated with the prefix 'apo' is greater than 5, in which case there is no need to give a Greek letter end-group designation for that end of the molecule.

Example:


H3C
CH3
CH3
CH3
CH3
CH3
H3C
H3C
CH3
CH3
16
17
19
20
18′
1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
15′
14′
13′
12′
11′
10′
9′
8′
7′
6′
5′
4′
3′
2′
1′
18
20′
19′
17′
16′

β,β-carotene
(fundamental parent structure)


H3C
CH3
CH3
CH3
CH3
CH3
CH3
CH3
16
17
19
20
1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
15′
14′
13′
12′
11′
10′
9′
8′
7′
6′
18
20′
19′

6′-apo-β-carotene
(see P-14.3.4 for use of unprimed and primed locants)

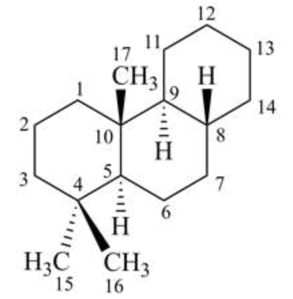
P-101.3.5 Bond migration

Parent structures that are not simple derivatives of accepted fundamental parents, but may be considered to arise from such parents by bond migration of one or more bonds, may be named by the following method.

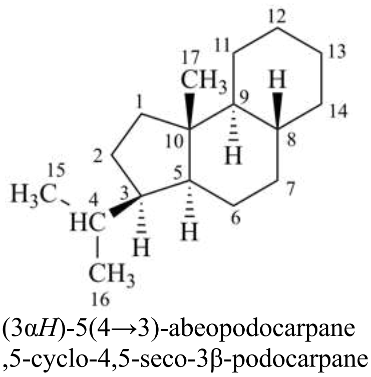
P-101.3.5.1 The nondetachable prefix '*x*(*y*→*z*)-abeo' designates the migration from one end of a single bond from its original position in a fundamental parent structure to another position. In the prefix, '*x*' is the locant of the stationary, i.e. unchanged, end of the migrating bond; '*y*' is the locant of the position of the moving end of the migrating bond in the parent structure; and 'z' is the locant of the position of the moving end in the final structure The numbering of the initial fundamental parent structure is retained.

Previously the prefix 'abeo' was italicized (Rule F-4.9, ref. 1; Rule R-1.2.7.1, ref. 2). For consistency with the other modifying prefixes it is now recommended that a regular roman font be used.

Example:


1
2
3
4
5
6
7
8
9
10
11
12
13
14
17
CH3
H
H
H
H3C
CH3
15
16

podocarpane
(fundamental parent structure)


1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17
CH3
H
H
H
H
H3C
HC
CH3

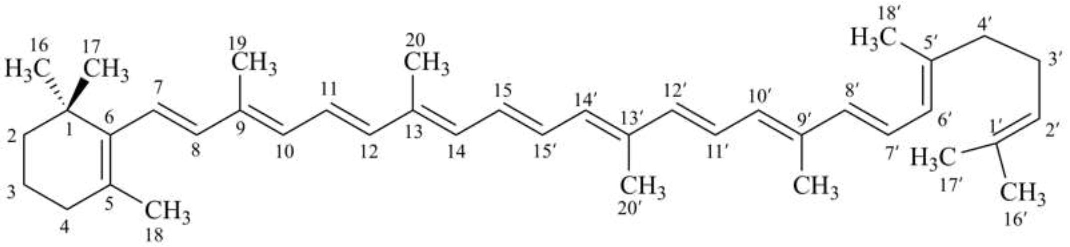
(3α*H*)-5(4→3)-abeopodocarpane
3,5-cyclo-4,5-seco-3β-podocarpane

The 'abeo' nomenclature described in this rule is permissive, not compulsory. It is most suitable for use in discussions on reaction mechanisms and biogenesis.

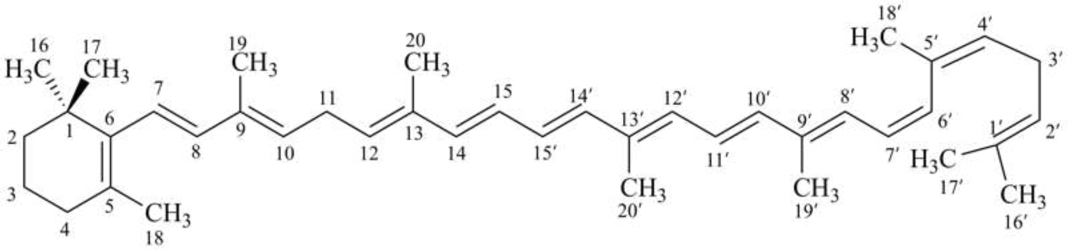
P-101.3.5.2 The italic prefix '*retro*' preceded by a pair of locants is used to indicate a shift, by one position, of all single and double bonds of a conjugated polyene system delineated by the pair of locants; the conjugated polyene system cannot be part of a system of maximum number of noncumulative double bonds in a ring or ring system. The first locant is the skeletal atom that has lost a hydrogen atom and the second locant the one that has gained a hydrogen atom.

The descriptor '*retro*' is used in this manner only in carotenoid nomenclature (see Carotenoid Rule 9, ref.9).

Example:



β,ψ-carotene (fundamental parent structure)

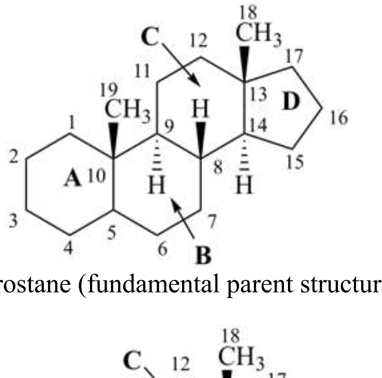


4′,11-*retro*-β,ψ-carotene
(see P-16.9 for use of primed and unprimed locants)

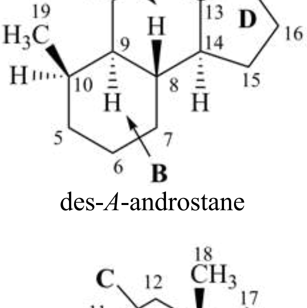
P-101.3.6 Removal of a terminal ring.

The removal of a terminal ring from a parent structure with the addition of an appropriate number of hydrogen atoms at each junction with the adjacent ring is indicated by the nondetachable prefix 'des' followed by the capital italic letter of the ring removed (see P-103.3.5.4 for use of 'des' in peptide nomenclature). This is the only time that the capital letters are now used to identify rings in a parent structure. Stereochemistry implied by the name of the stereoparent structure remains the same, unless otherwise specified. Numbering of skeletal atoms of the parent structure is retained in the modified structure. This use of 'des' is restricted to steroids.

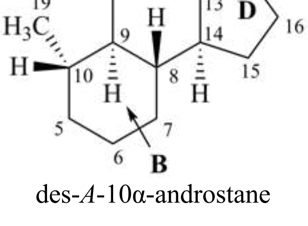
Example:



androstane (fundamental parent structure)



des-*A*-androstane



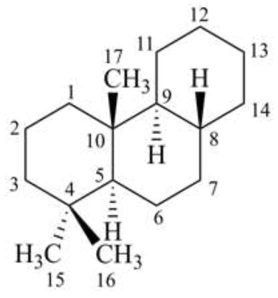
des-*A*-10α-androstane

P-101.3.7 Combination of the prefixes ‘cyclo’, ‘seco’, ‘apo’, ‘homo’, and ‘nor’

Modifications to a fundamental parent structure prescribed by the prefixes in the preceding recommendations (P-101.3.1 through P-101.3.4) may be combined to effect even more drastic changes in structure. The operation indicated by each prefix ‘cyclo’, ‘seco’, ‘apo’, ‘homo’, and ‘nor’ is applied to the fundamental parent structure sequentially as one ‘advances backward’, i.e. moves from right to left from the name of the fundamental parent structure.

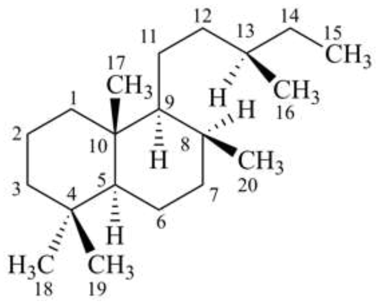
P-101.3.7.1 When different combinations of prefixes ‘cyclo’, ‘seco’, ‘apo’, ‘homo’, and ‘nor’ can be used to effect the same transformation in fundamental parent structure, the combination of choice must express the fewest number of operations. Both detachable (e.g. alkyl) and nondetachable (e.g. homo or nor) prefixes are considered as modifications but detachable prefixes are preferred. Dihomo, dinor, etc., are counted as two modifications each (see ref. 16, Rule 3S-6.3). When the number of operations is the same, the combination of homo/nor is preferred to cyclo/seco; choice between other combinations expressing the same number of operations is based on earlier alphabetical order of the prefixes.

Examples:



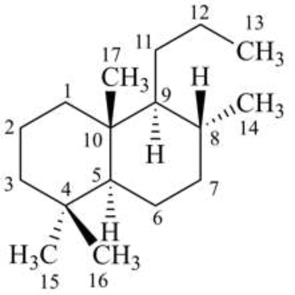
17
CH3
H
H
H
H3C
CH3
15
16
1 2 3 4 5 6 7 8 9 10 11 12 13 14

podocarpane
(fundamental parent structure)



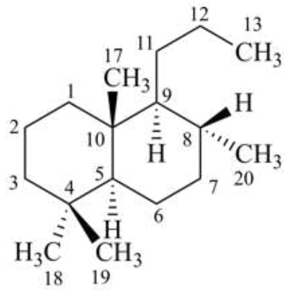
17
CH3
H
H
H
H
CH3
16
CH3
20
CH3
15
H3C
CH3
18
19
1 2 3 4 5 6 7 8 9 10 11 12 13 14

labdane
(fundamental parent structure)



17
CH3
H
CH3
14
CH3
13
H
H
H3C
CH3
15
16
1 2 3 4 5 6 7 8 9 10 11 12

≡

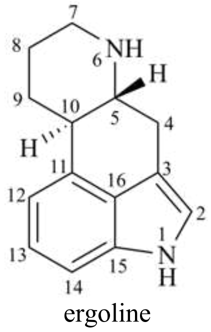


17
CH3
H
CH3
20
CH3
13
H
H
H3C
CH3
18
19
1 2 3 4 5 6 7 8 9 10 11 12

(**I**) (**II**)

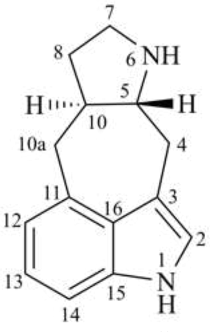
13,14-secopodocarpane (**I**) not 8α-14,15,16-trinorlabdane (**II**)

Explanation: Podocarpane may be used to generate the ‘seco’ compound with one operation; the same compound may be obtained from labdane but in three operations.



NH
H
H
N
H
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16

ergoline
(fundamental parent structure)



NH
H
H
N
H
10a
1 2 3 4 5 6 7 8 10 11 12 13 14 15 16

10(11)a-homo-9-norergoline (preferred)
5,9-cyclo-5,10-secoergoline
(9*H*)-5(10→9)-abeoergoline

P-101.3.7.2 The order of citation of combinations of structure modifying prefixes must avoid improper use of the prefixes as defined above or impossible situations when the corresponding operations are carried out in the manner prescribed above.

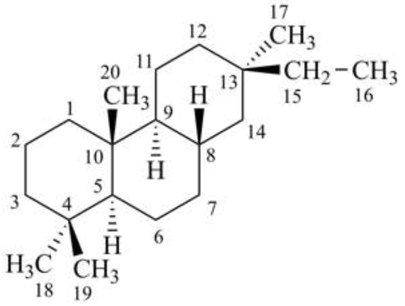
After satisfying P-101.3.7.1 and P-101.3.7.2, the nondetachable prefixes that indicate bond rearrangements (‘cyclo’ and ‘seco’) are cited, followed by those that indicate addition or removal of skeletal atoms (‘homo’ and ‘nor’). If more than one of any of these operations is needed, they are cited in alphabetical order before the name of the fundamental parent structure. Multiplying prefixes denoting multiple operations of the same kind do not affect the order.

The preferred semisystematic name results from modifications by only two operations involving the prefixes ‘cyclo’, ‘seco’, ‘apo’, ‘homo’, and ‘nor’. In general nomenclature, more than two operations are allowed. Names are formed by citing the bond rearrangement prefixes ‘cyclo’ and ‘seco’, first, (farthest from the parent structure) in that order from left to right, followed by the removal/addition prefixes ‘homo’ and ‘nor, in that order from left to right, at the front of the name of the parent structure. Schematically this order is as follows:

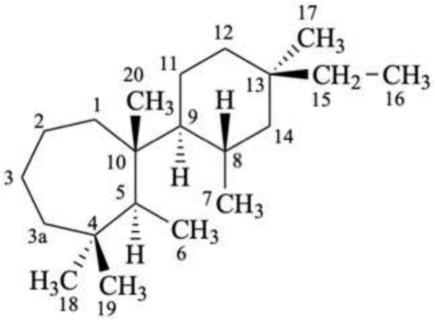
operation	bond rearrangement	addition/removal of skeletal atoms	parent structure
	cyclo, seco	apo, homo, nor	

Names in which the order of prefixes is cyclo/seco/apo/homo/nor are preferred to those denoted by the alphabetical order apo/cyclo/homo/nor/seco for the five prefixes.

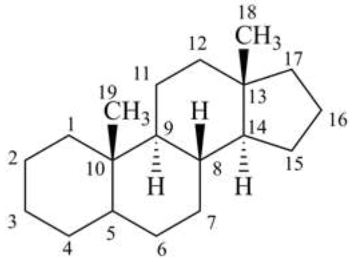
Examples:


17
CH3
12
11
20
13
CH2−CH3
15
16
CH3
9
H
1
14
2
10
8
H
5
3
4
7
H
6
H3C
CH3
18
19

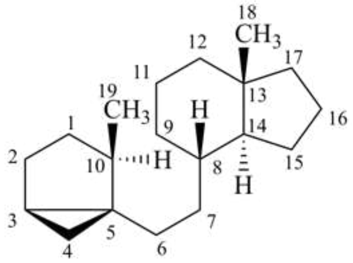
pimarane
(fundamental parent structure)


17
CH3
12
11
20
13
CH2−CH3
15
16
CH3
9
H
1
2
14
10
8
H
3
5
7
CH3
CH3
3a
4
H
6
H3C
CH3
18
19

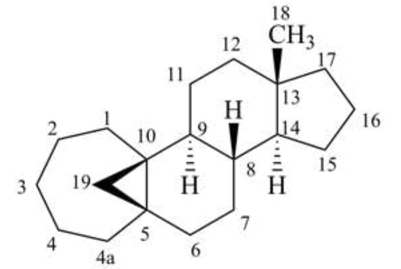
6,7-seco-3a-homopimarane (preferred)
3a-homo-6,7-secopimarane

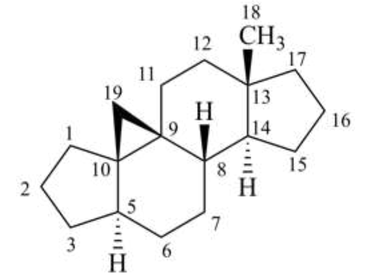

18
CH3
12
17
11
13
19
CH3
16
H
1
9
14
2
10
8
15
H
H
3
5
7
4
6

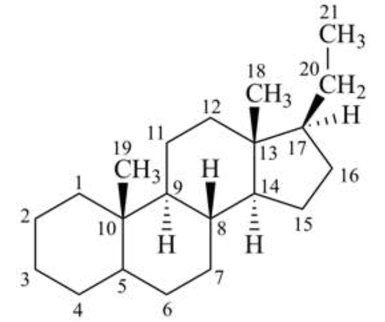
androstane
(fundamental parent structure)

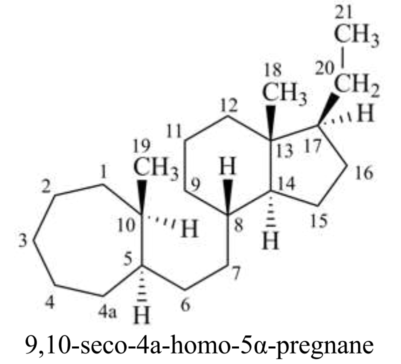

18
CH3
12
17
11
19
13
CH3
16
9
H
1
14
2
10
H
8
15
H
3
5
7
4
6

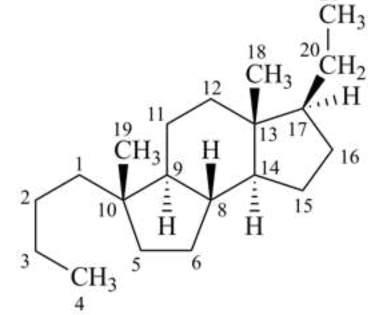
3α,5α-cyclo-9,10-seco-5α-androstane

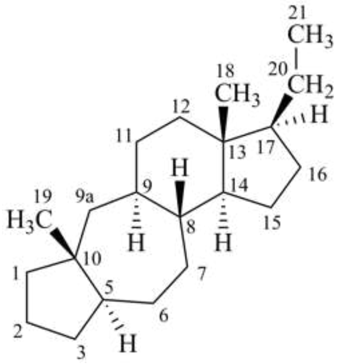

5β,19-cyclo-4a-homo-5β-androstane


9β,19-cyclo-4-nor-5α,9β-androstane


pregnane
(fundamental parent structure)


9,10-seco-4a-homo-5α-pregnane


4,5-seco-7-norpregnane


9a-homo-4-nor-5α-pregnane

P-101.4 REPLACEMENT OF SKELETAL ATOMS

P-101.4.1 General methodology
P-101.4.2 Skeletal replacement of carbon atoms by heteroatoms
P-101.4.3 Skeletal replacement of heteroatoms by carbon atoms
P-101.4.4.Skeketal replacement of heteroatoms by other heteroatoms
P-101.4.5 Indicated hydrogen

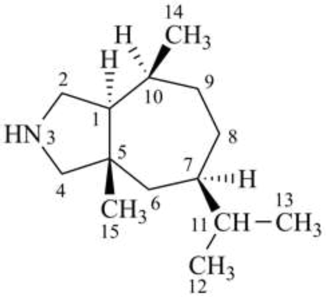
P-101.4.1 General methodology

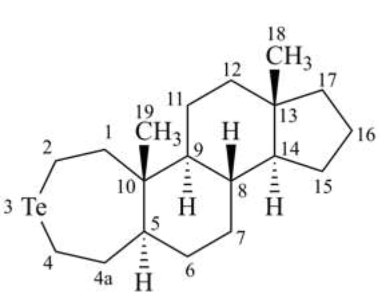
The principles of skeletal replacement ('a') nomenclature, as described in P-15.4 and P-51.4 to modify parent structures, are applied to replace carbon skeletal atoms by heteroatoms, such as O, S, N. Contrary to the recommended alphabetical order for citation in names in the Revised Section F (ref. 9), the seniority order of the 'a' prefixes prescribed in P-15.4 is recommended for skeletal replacement. In addition to the methodology used to generate systematic names, skeletal replacement ('a') nomenclature is also used to replace heteroatoms in parent structures by carbon atoms and by other heteroatoms.

P-101.4.2 Skeletal replacement of carbon atoms by heteroatoms

Heteroatoms are denoted by 'a' prefixes that are cited before nondetachable prefixes expressing skeletal modifications in fundamental parent structures, each with a locant to indicate its position; the fixed numbering of the parent structure is maintained. Skeletal modifications, if any, must be completed before skeletal replacement ('a') nomenclature can be applied.

Examples:

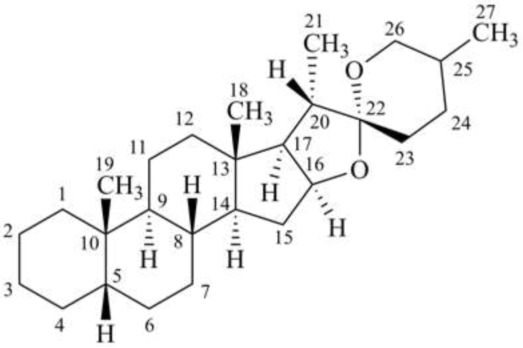

3-azaambrosane


3-tellura-4a-homo-5α-androstane

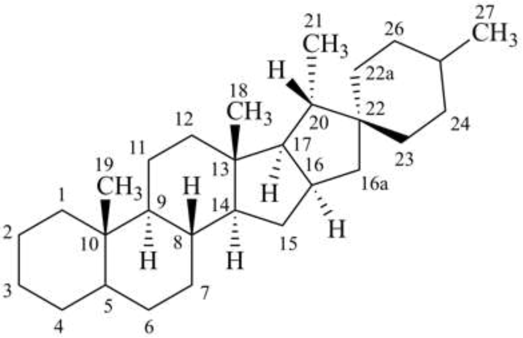
P-101.4.3 Skeletal replacement of heteroatoms by carbon atoms

Replacement of a heteroatom in a parent structure by a carbon atom is indicated by the replacement ('a') prefix 'carba'. The original numbering is maintained. If the heteroatom is not numbered, the replacing carbon atom is numbered by affixing the letter 'a' to the locant of the immediately adjacent lower numbered skeletal atom. If the immediately adjacent lower numbered skeletal atom is a 'homo' atom, the letter 'b', 'c', etc., as appropriate, is used. Configuration at the new carbon skeletal atom is described by methods for specifying additional configuration (see P-101.2.6.1).

Examples:



spirostan
(fundamental parent structure)

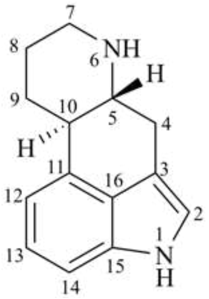


16a,22a-dicarba-5β-spirostan

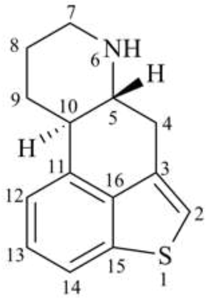
P-101.4.4 Skeletal replacement of heteroatoms by other heteroatoms

Replacement of a heteroatom in a stereoparent hydride by another heteroatom is denoted by the appropriate skeletal replacement ('a') prefix and locant.

Example:



ergoline
(fundamental parent structure)

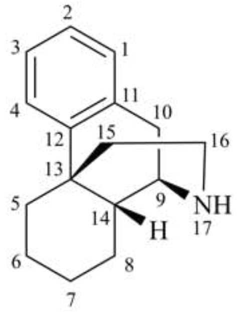


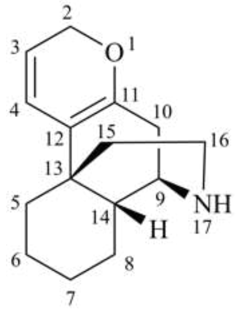
1-thiaergoline

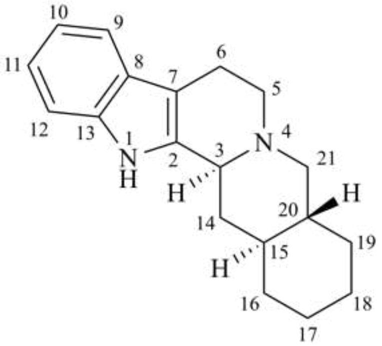
P-101.4.5 Indicated hydrogen

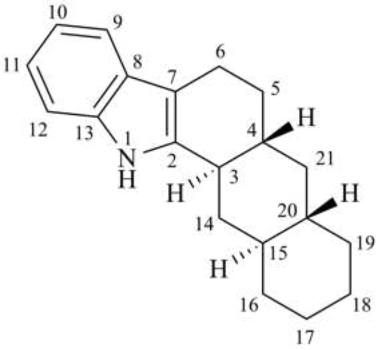
When the replacement of a skeletal atom in a portion of a parent structure that is mancude (contains the maximum number of noncumulative double bonds) or an extended conjugated system of double bonds results in the creation of a saturated skeletal position, that position is indicated by the symbolism of indicated hydrogen (see P-14.7 and P-58.2).

Examples:


morphinan
(fundamental parent structure)


2*H*-1-oxamorphinan


yohimban
(fundamental parent structure)


(4β*H*)-4-carbayohimban

P-101.5 ADDITION OF RINGS AND RING SYSTEMS

Three types of rings and ring systems can be incorporated into parent structures:

P-101.5.1 Mancude rings and ring systems incorporated by fusion nomenclature
P-101.5.2 Rings and ring systems incorporated by bridged fused ring nomenclature
P-101.5.3 Rings and ring systems incorporated by spiro nomenclature

The methods, in certain cases adapted to parent structures, used for the construction of systematic names and described in Chapters P-1 through P-8 above, are applied.

P-101.5.1 Mancude rings and ring systems incorporated by fusion nomenclature

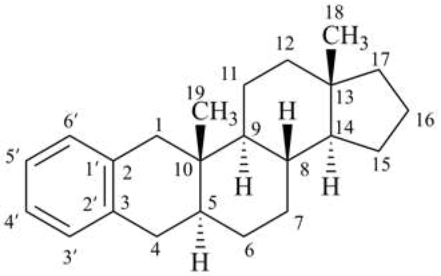
The fundamental parent structure as a component is used in fusion nomenclature in its normal state of hydrogenation. Accordingly, a double bond is not cited at the fusion site just because the other component contains the maximum of noncumulative double bonds. Furthermore, contrary to the rules prescribed in P-25, a fundamental parent structure is always chosen as the principal component and the attached component must be a mancude ring or ring system.

P-101.5.1.1 A ring or ring system considered as a mancude parent hydride in accordance with the rules prescribed in Chapter P-2, carbocyclic or heterocyclic, fused to a parent structure is described by its fusion prefix name (see P-25) preceding the name of the fundamental parent structure. The skeletal atoms of the parent structure involved in the fusion are identified by plain (unprimed) locants and not by italicized letters ‘a’, ‘b’, etc.; the skeletal atoms of the mancude component, involved in the fusion, are identified by primed locant numbers. The position of the fusion is indicated by a fusion descriptor, including two sets of locants; the first cited set is that of the attached component, the second set relates to the principal component, the fundamental parent structure; the two sets are separated by a colon, enclosed in brackets, and cited between the two components. Where there is a choice, the locants for the mancude attached component are as low as possible and are cited in the same direction of numbering as for the parent structure.

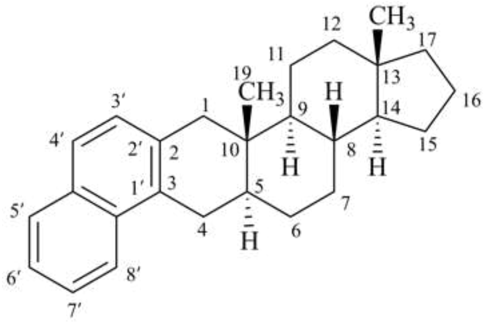
Terminal vowels, ‘o’ or ‘a’, in the name of the prefix are not elided when followed by a vowel, as prescribed for normal fusion nomenclature in P-25.3.1.3.

No elision of vowels is a change from previous recommendations.

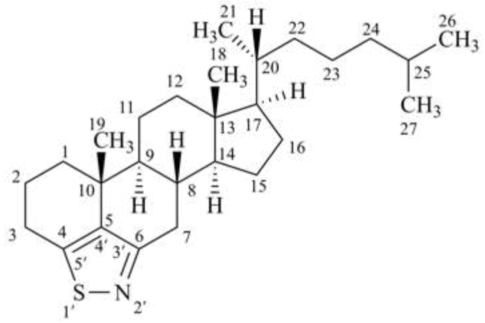
Examples:



benzo[2,3]-5α-androstane
(locants 1′,2′ are omitted)



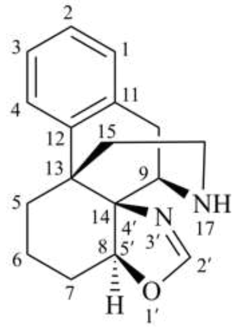
naphtho[2′,1′:2,3]-5α-androstane

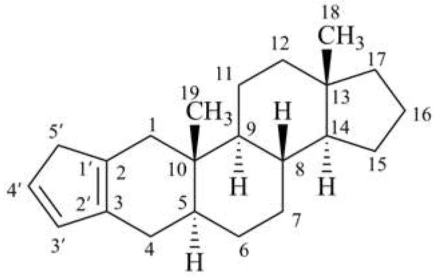


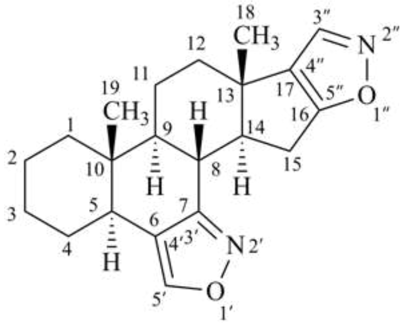
[1,2]thiazolo[5′,4′,3′:4,5,6]cholestane
(not isothiazolo[5′,4′,3′:4,5,6]cholestane;
the name isothiazole is no longer recommended as a fusion component, see P-25.3.2.1.2)

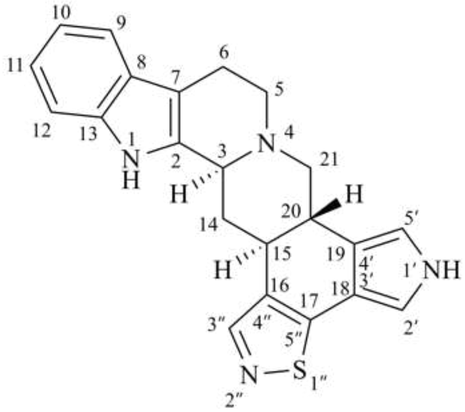
P-101.5.1.2 The attached component fused to a parent structure is a mancude compound (it contains the maximum number of noncumulative double bonds). Saturated positions on such components, including the fusion sites, that have at least one hydrogen atom are specified by an indicated hydrogen. They are also specified by a descriptor composed of the locant, followed by the configuration descriptor ‘α’ or ‘β’ and finally by the indicated hydrogen symbolism (see P-14.7), placed in parentheses at the front of the name as are stereodescriptors. Locants of the attached component are used to identify the position of the indicated hydrogen, but locants (unprimed) of the stereoparent hydride are used, if there is a choice between primed and unprimed locants.

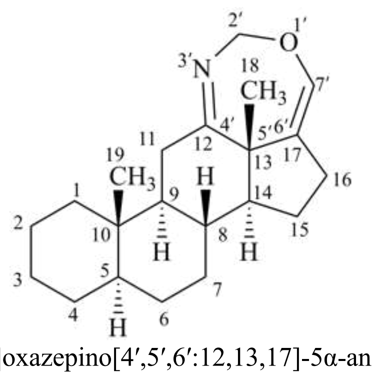
Examples:

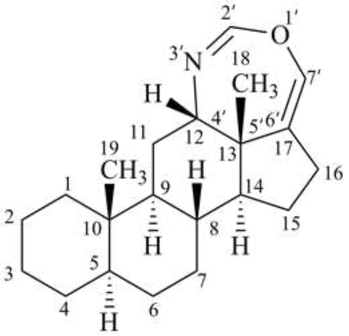

(8α*H*)-[1,3]oxazolo[5′,4′:8,14]morphinan
[not 8α*H*-oxazolo[5′,4′:8,14]morphinan;
the name oxazole without heteroatom locants is no longer recommended as a fusion component;
an ‘indicated hydrogen atom’ denoted by the stereodescriptor (8α*H*) is needed to complete the name]


5′*H*-cyclopenta[2,3]-5α-androstane


bis[1,2]oxazolo[4′,3′:6,7;5″,4″:16,17]-5α-androstane


1′*H*-pyrrolo[3′,4′:18,19][1,2]thiazolo[4″,5″:16,17]yohimban


2′*H*-[1,3]oxazepino[4′,5′,6′:12,13,17]-5α-androstane

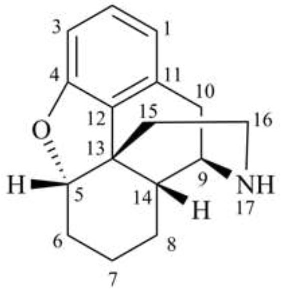

2′
1′
3′N
O
18
CH3
7′
H
4′
5′6′
11
12
19
CH3
13
17
16
1
9
H
14
2
10
8
15
H
H
5
3
7
4
6
H

(12β*H*)-12*H*-[1,3]oxazepino[4′,5′,6′:12,13,17]-5α-androstane

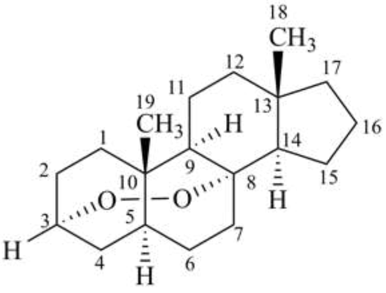
P-101.5.2 Rings and ring systems incorporated by bridged fused ring nomenclature

Atomic bridges added to fundamental parent structures may be described by the methods used in fusion nomenclature for bridged fused ring systems. The names of the bridges are those prescribed in P-25.4. This method is often used with heteroatom bridges. In fact, this method is often more useful than fusion procedures described in P-101.5.1 for describing certain types of heterocyclic rings fused to a fundamental parent structure, for instance 'epoxy' to denote a bridge rather than 'oxireno' to denote the ring fused as an attached component. The use of atomic bridges is preferred to fusion nomenclature to connect two nonadjacent atoms in a fundamental parent structure [epoxides and thioepoxides are exceptions as they can be named substitutively (see P-63.5)]. The prefixes used to denote bridges are nondetachable; they are cited in a name in front of the prefixes used to denote skeletal modifications, preceded by appropriate locants.

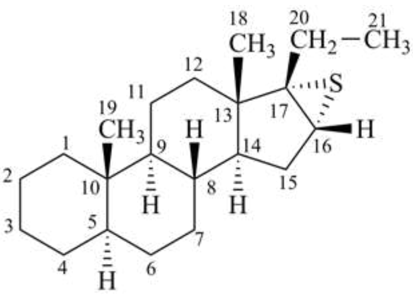
Examples:


2
3
1
4
11
10
O
12
15
16
13
H
5
9
NH
14
H
17
6
8
7

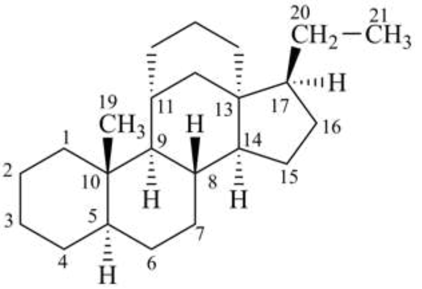
4,5α-epoxymorphinan
(5β*H*)-5,13-dihydrofuro[2′,3′,4′,5′:4,12,13,5]morphinan


18
CH3
12
17
11
19
13
CH3
H
16
1
14
9
2
10
8
15
O
O
H
3
5
7
H
4
6
H

3α,8-epidioxy-5α,8α-androstane

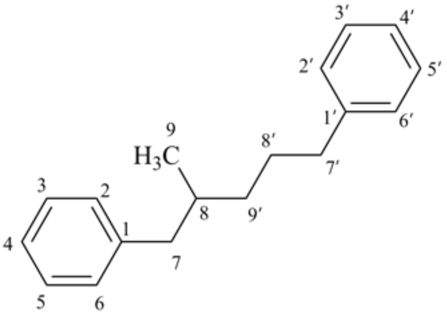

18
20
21
CH3
CH2−CH3
12
S
11
17
19
13
H
CH3
H
16
1
9
14
2
10
8
15
H
H
5
3
7
4
6
H

(16β*H*)-thiireno[2′,3′:16,17]-5α-pregnane (fusion name)
16α,17-epithio-5α-pregnane

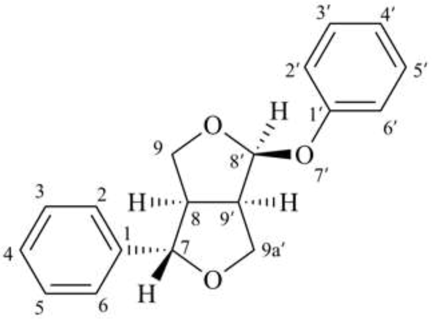


11α,18-ethano-5α,13α-pregnane
11α,13-propano-18-nor-5α,13α-pregnane
11β,18-cyclo-12a,12b-dihomo-5α-pregnane
11α,18b-cyclo-18a,18b-dihomo-5α,13α-pregnane

Explanation: The inversion of configuration at C-13 is not counted as an operation since it is not modifying the skeleton of the molecule.



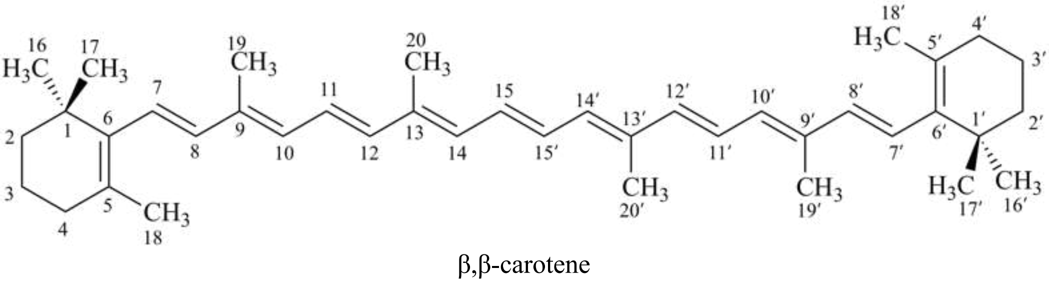
8,9′-neolignane
(fundamental parent structure)
1,1′-(2-methylpentane-1,5-diyl)dibenzene



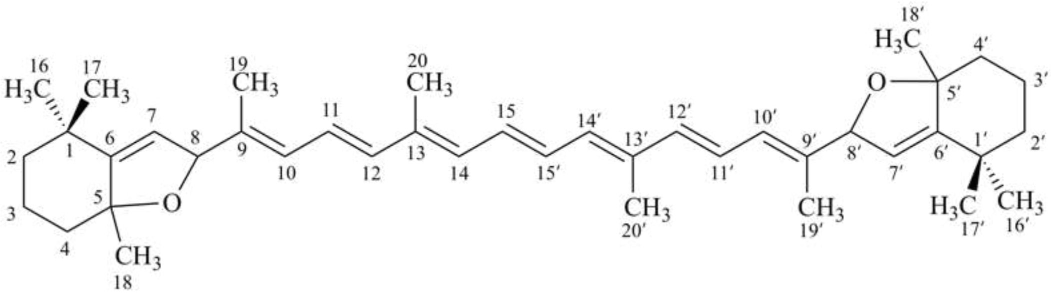
(7α,8α,8′β,9′α)-7,9a′:8′,9-diepoxy-7′-oxa-9a′-homo-8,9′-neolignane
(1*S*,3a*R*,4*S*,6a*R*)-1-phenoxy-4-phenyltetrahydro-1*H*,3*H*-furo[3,4-*c*]furan

Contrary to the recommendations for systematic nomenclature of organic compounds, in carotenoid nomenclature (see ref. 40), the bridge named ‘epoxy’ is considered detachable and the hydro/dehydro prefixes nondetachable. The name of the following bridged β,β-carotene is written in conformity with the rules of carotenoid nomenclature (ref. 40, Carotenoid Rule 7.3) but in contradiction to Rule P-15.1.5.

Examples:



β,β-carotene
(fundamental parent structure)

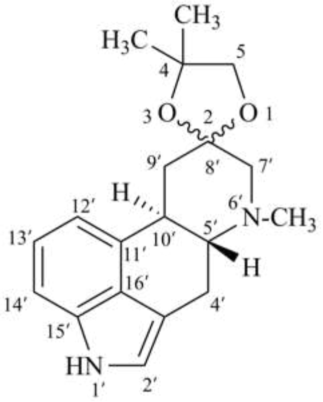


5,8:5′,8′-diepoxy-5,8,5′,8′-tetrahydro-β,β-carotene
(see P-14.3.1 for use of unprimed and primed locants)

P-101.5.3 Rings and ring systems incorporated by spiro nomenclature

Spiro compounds are named as prescribed in P-24.5 for monospiro compound having at least one polycyclic component.

Example:



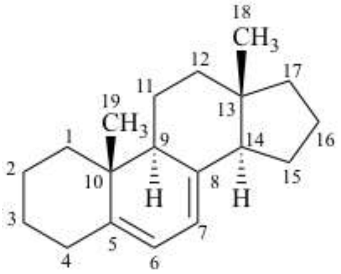
(2ξ)-4,4,6′-trimethylspiro[1,3-dioxolane-2,8′-ergoline]

P-101.6 MODIFICATION OF THE DEGREE OF HYDROGENATION OF PARENT STRUCTURES

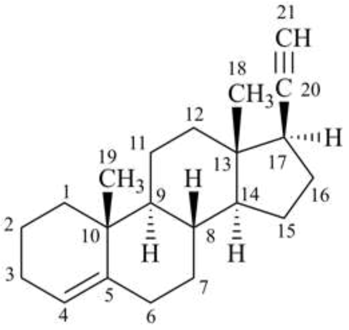
The general principles and rules for modifying the degree of hydrogenation of parent hydrides prescribed in Section P-31 are applied to parent structures. The endings ‘ene’ and ‘yne’ (see P-31.1) and the prefixes ‘hydro’ and ‘dehydro’ (see P-31.2) are used, depending on the subtractive or additive operation required. There is no limit to the introduction of double bonds in parent hydrides; ‘hydro/dehydro’ prefixes can be used in any number, as required, provided that no mancude structure is generated.

P-101.6.1 Unsaturation in a compound whose parent structure is fully saturated or in the portion of a parent structure that is otherwise fully saturated and whose name ends in ‘an’, ‘ane’, or ‘anine’ is indicated by changing ‘an’ or ‘ane’ to ‘ene’ or ‘yne’ and ‘anine’ to ‘enine’ or ‘ynine’ and by adding numerical multiplying prefixes as prescribed in P-31.1.1.2. Locants are placed immediately before the part of the name to which they relate.

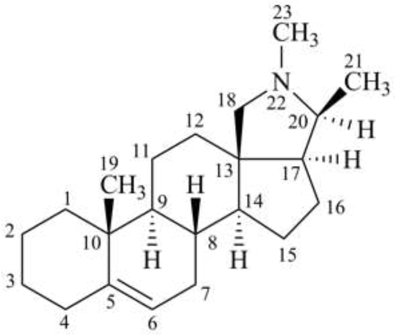
Examples:



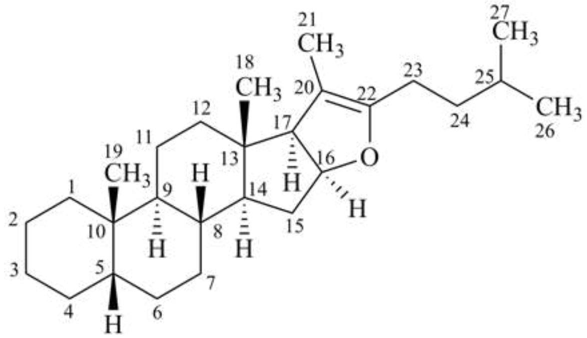
androsta-5,7-diene



pregn-4-en-20-yne



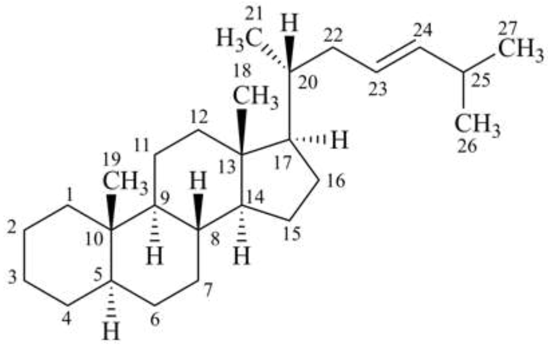
con-5-enine



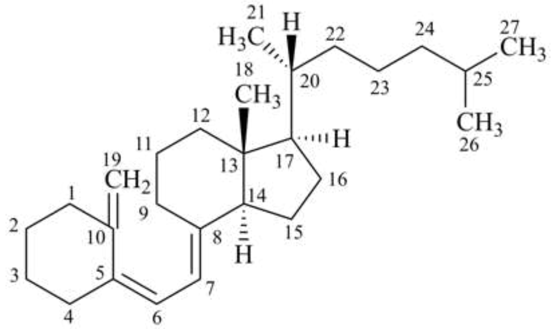
5β-furost-20(22)-ene

P-101.6.2 The descriptors '*E*' and '*Z*', preceded by appropriate locants, are used to describe modified or additional stereochemical configurations for double bonds. The stereodescriptors '*cis*' and '*trans*' are used in carotenoid nomenclature (ref. 40) and retinoid nomenclature (ref. 49).

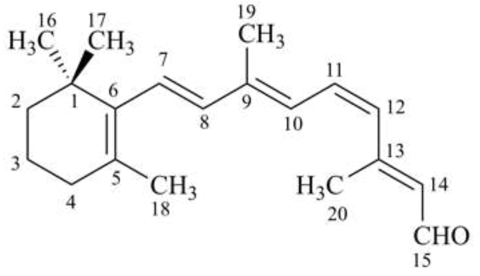
Examples:



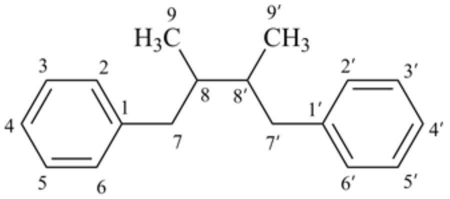
(23*E*)-5α-cholest-23-ene



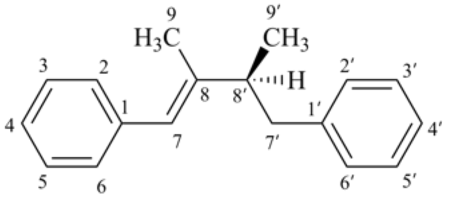
(5*Z*,7*E*)-9,10-secocholesta-5,7,10(19)-triene



11-*cis*-retinal



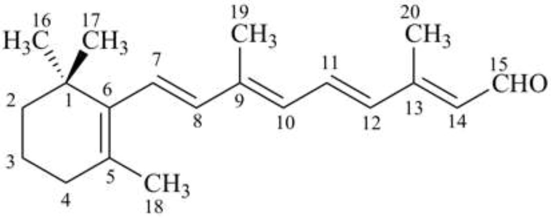
lignane
(fundamental parent structure)



(7*E*,8′*S*)-lign-7-ene
[(1*E*,3*S*)-2,3-dimethyl-4-phenylbut-1-en-1-yl]benzene
1,1′-[(1*E*,3*S*)-(2,3-dimethylbut-1-ene-1,4-diyl)]dibenzene

P-101.6.3 The prefix '*all*' is used in front of stereodescriptors to indicate that all configurations are identical. This prefix is used only in the nomenclature of natural products, for example, '*all-trans*' to denote the fact that in retinal all double bonds are '*trans*'.

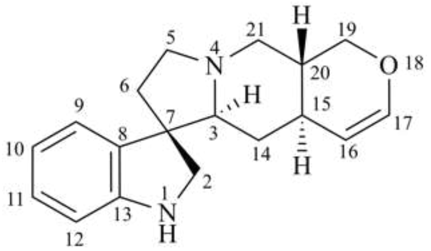
Example:



all-trans-retinal

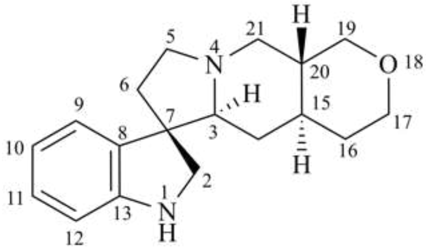
P-101.6.4 Saturation of double bonds in a parent structure whose name implies the presence of isolated double bonds and/or systems of conjugated double bonds is described by the prefix 'hydro', itself preceded by the locants of the saturated positions. The ‘hydro’ prefix is detachable and always cited immediately in front of the fundamental parent structure (see P-31.2).

Examples:



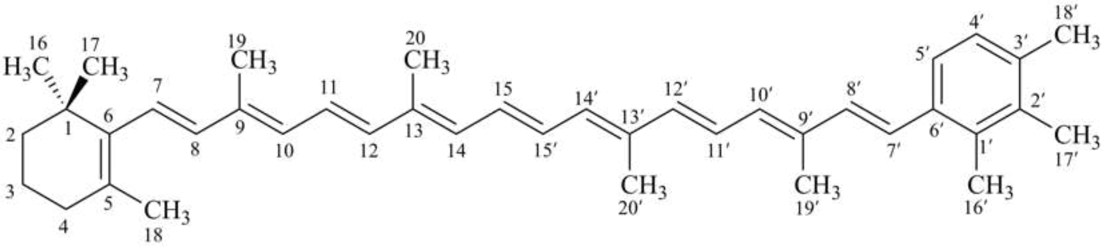
H
21
19
5
4
N
20
O
18
6
H
15
9
7
3
17
10
8
14
16
H
2
11
1
13
N
H
12

formosanan
(fundamental parent structure)



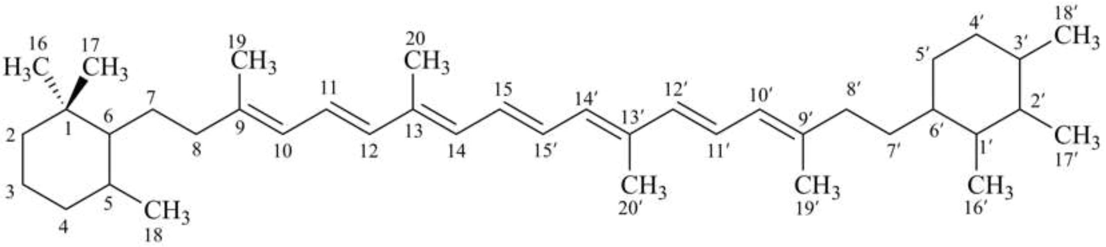
H
21
19
5
4
N
20
O
18
6
H
15
9
7
3
17
10
8
16
H
2
11
1
13
N
H
12

16,17-dihydroformosanan



16
17
H_3C
CH_3
19
CH_3
20
CH_3
4′
18′
CH_3
5′
3′
7
11
15
14′
12′
10′
8′
2′
6
9
13
13′
9′
6′
2
1
8
10
12
14
15′
11′
7′
1′
CH_3
17′
3
5
CH_3
CH_3
CH_3
CH_3
4
18
20′
19′
16′

β,χ-carotene

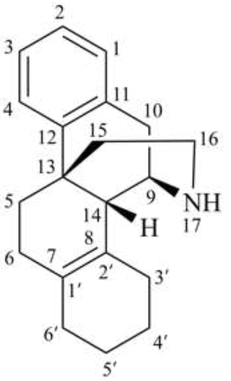


16
17
H_3C
CH_3
19
CH_3
20
CH_3
4′
18′
CH_3
5′
3′
7
11
15
14′
12′
10′
8′
2′
6
9
13
13′
9′
6′
2
1
8
10
12
14
15′
11′
7′
1′
CH_3
17′
3
5
CH_3
CH_3
CH_3
CH_3
4
18
20′
19′
16′

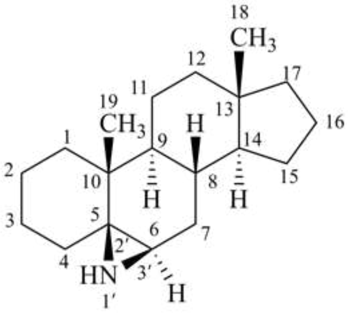
5,6,7,8,1′,2′,3′,4′,5′,6′,7′,8′-dodecahydro-β,χ-carotene
(see P-14.3.1 for use of unprimed and primed locants)

P-101.6.5 Saturated, or partially saturated, carbocyclic and heterocyclic ring components fused to a parent structure are named using ‘hydro’ prefixes. When there is a choice between primed and unprimed locants, the unprimed locants are used.

Examples:



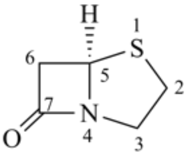
3′,4′,5′,6′-tetrahydrobenzo[7,8]morphinan



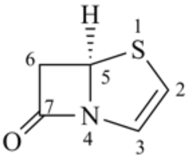
(6α*H*)-1′,6-dihydroazirino[2′,3′:5,6]-5β-androstane
[for the symbol (6α*H*), see P-101.5.1.2]

P-101.6.6 The introduction of unsaturation additional to any unsaturation implied in a parent structure whose name does not end in 'an', 'ane', or 'anine', the conversion of an implied double bond into a triple bond, and the introduction of an additional double bond with rearrangement of an implied double bond are denoted by the prefix 'dehydro', itself prefixed by a numerical multiplying term equal to the number of hydrogen atoms removed and the appropriate locants. The 'dehydro' prefix is detachable and always cited at the front of the fundamental parent structure, after any detachable alphabetized prefixes, when present.

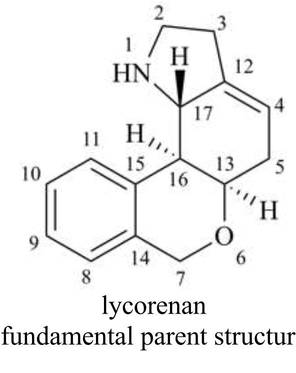
Examples:



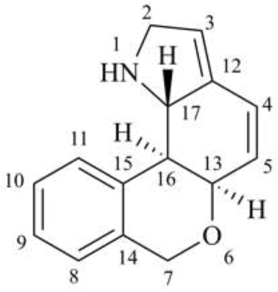
penam
(fundamental parent structure)
(note new numbering)



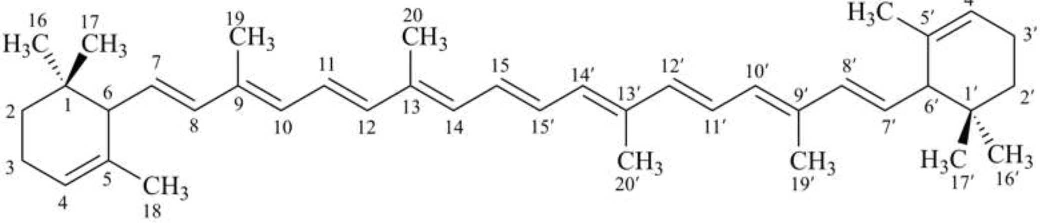
2,3-didehydropenam



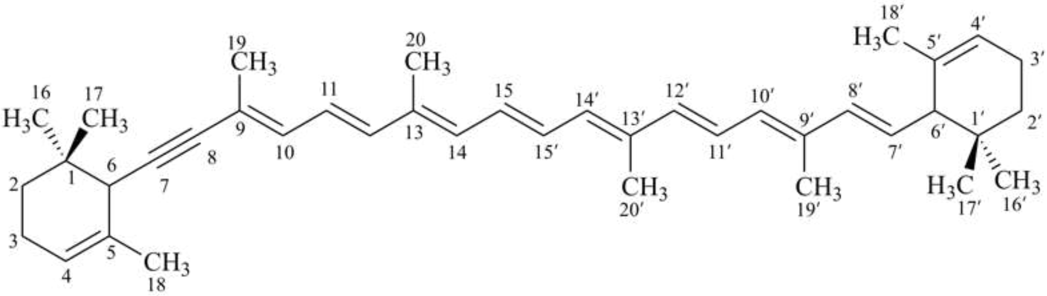
lycorenan
(fundamental parent structure)



3,5-didehydrolycorenan



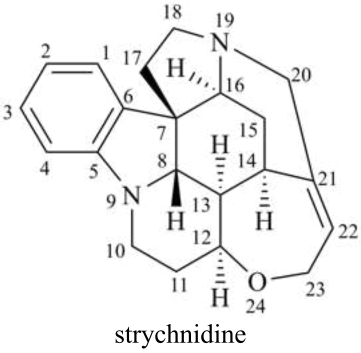
ε,ε-carotene
(fundamental parent structure)



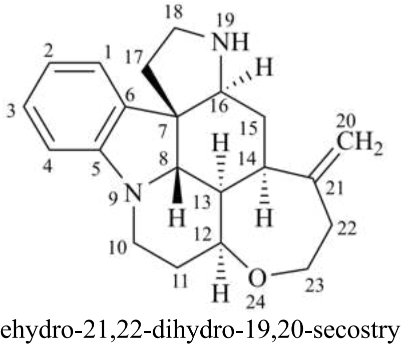
7,8-didehydro-ε,ε-carotene
(see Rule P-14.3.1 for use of unprimed and primed locants)

P-101.6.7 Rearrangement of double bonds may be indicated by a combination of 'hydro' and 'dehydro' prefixes. The 'dehydro' prefix is cited before the 'hydro' prefix, in accordance with the alphanumerical order.

Example:



strychnidine
(fundamental parent structure)



20,21-didehydro-21,22-dihydro-19,20-secostrychnidine

P-101.7 DERIVATIVES OF PARENT STRUCTURES

Derivatives of parent structures are named according to principles, rules, and conventions described in Chapters P-1 through P-9.

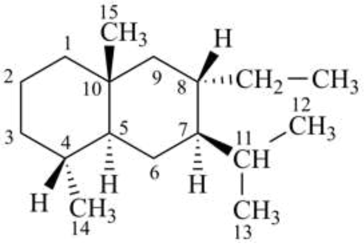
P-101.7.1 The suffixes and prefixes of the nomenclature of organic compounds are used in the prescribed manner to name atoms and groups that are considered to substitute for hydrogen atoms of parent structures. The stereodescriptors α, β, and ξ are used to describe the configuration; they are cited in front of the prefix or suffix, preceded by the appropriate locant. Substitutive names so constructed are preferred to those that are formed by functional class nomenclature, except for some cyclic functional classes.

Substitution on rings and substitution on terminal segments are considered separately.

P-101.7.1.1 Substitution by alkyl groups

P-101.7.1.1.1 Organyl groups such as aryl groups and alkyl groups are introduced by substitutive nomenclature.

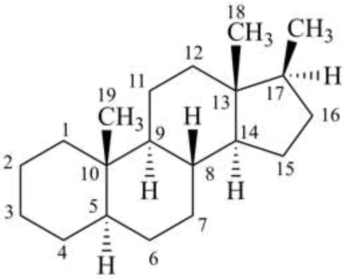
Example:


15
CH3
H
1
2
3
4
5
6
7
8
9
10
CH2−CH3
12
CH3
11
CH
H
H
H
CH3
14
CH3
13

8α-ethyleudesmane

P-101.7.1.1.2 The substitutive procedure is used to introduce a methyl group in androstane at position 17β; the alternative method of subtracting a methylene group from pregnane by using the nondetachable prefix ‘nor’ is not recommended (see P-101.3.7.1).

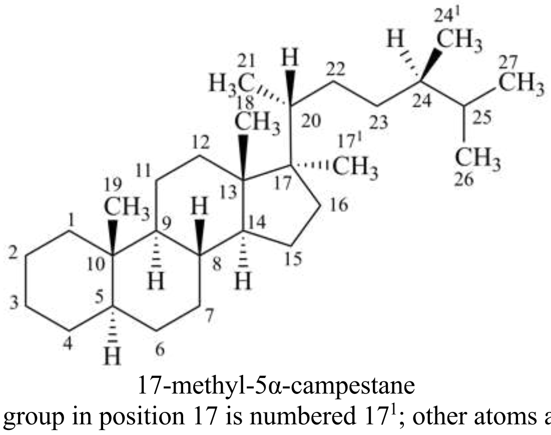
Example:


18
CH3
CH3
H
12
11
13
17
16
19
CH3
H
9
14
1
2
10
8
15
H
H
3
5
7
4
H
6

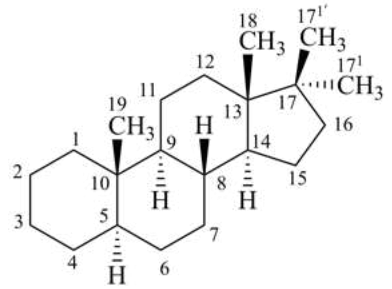
17β-methyl-5α-androstane
(not 21-nor-5α-pregnane)

P-101.7.1.1.3 Rule 3S-2.7 in ref. 16 describes the methodology to name steroids with a side chain as part of the parent carbocycle and an alkyl substituent at C-17. Rule 3S-2.7 also describes the methodology to name steroids with two alkyl substituents at C-17. This methodology is applicable to any fundamental parent structure described in Section P-101. Locants with superscript numbers are intended for the identification of the atoms, e.g. in ^{13}C-nmr assignments, not as locants for further substitution.

Examples:


24¹
H
CH3
21
H
22
27
H3C
CH3
18
24
25
CH3
20
23
12
17¹
CH3
CH3
11
13
17
26
19
16
CH3
H
1
9
14
2
10
8
15
H
H
3
5
7
4
H
6

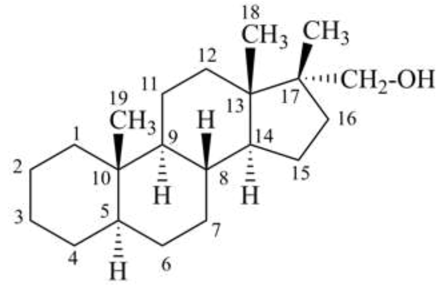
17-methyl-5α-campestane
(the additional methyl group in position 17 is numbered 17^1; other atoms are numbered as usual)



17,17-dimethyl-5α-androstane
(both additional methyl groups are numbererd 17^1; the β-methyl group is primed)

P-101.7.1.1.4 The principles, rules, and conventions of substitutive nomenclature are used when a characteristic group cited as a suffix is present on an alkyl substituent group added to a fundamental parent structure.

Example:

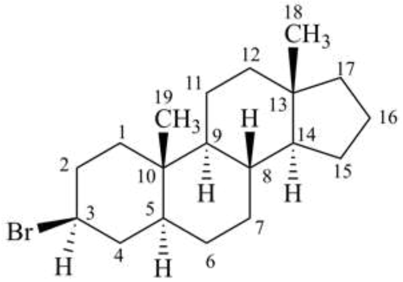


(17β-methyl-5α-androstan-17α-yl)methanol
[not (21-nor-5α-pregnan-17α-yl)methanol]

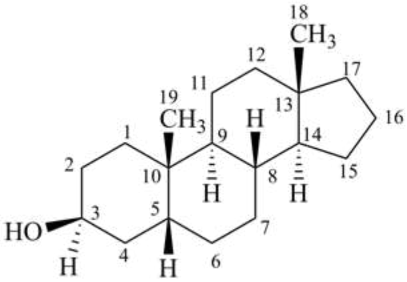
P-101.7.1.2 Substitution on rings

Suffixes are used in accordance with the seniority order of suffixes, considering the cyclic nature of the parent hydride. Detachable prefixes are cited in alphanumerical order. The endings ‘ene’ and ‘yne’ are cited in the normal way; the ‘hydro-dehydro’ prefixes are detachable but cited last among detachable prefixes.

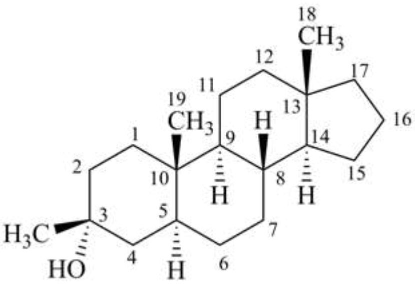
Examples:



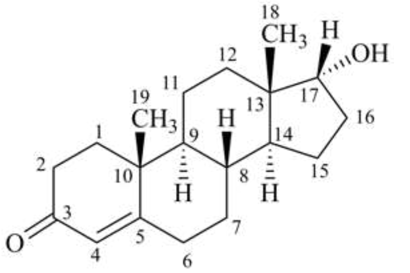
3β-bromo-5α-androstane
5α-androstan-3β-yl bromide



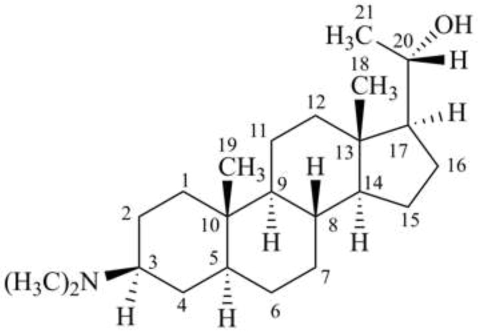
5β-androstan-3β-ol



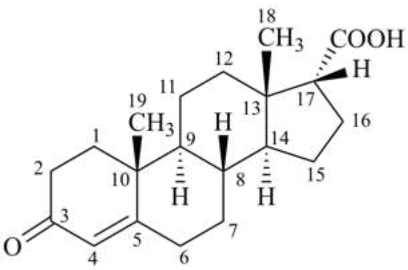
3β-methyl-5α-androstan-3α-ol



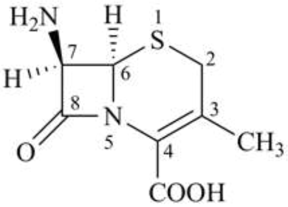
17α-hydroxyandrost-4-en-3-one



(20*S*)-3β-(dimethylamino)-5α-pregnan-20-ol



3-oxoandrost-4-ene-17α-carboxylic acid
[not 21-nor-5α-pregnan-20-oic acid;
the correct name involves the fewest number of operations (see P-101.3.7.1)]

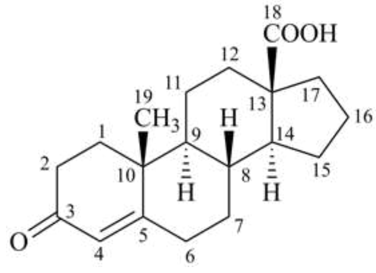


(6*R*,7*R*)-7-amino-3-methyl-8-oxo-5-thia-1-azabicyclo[4.2.0]oct-2-en-2-carboxylic acid
7β-amino-3-methyl-3,4-didehydrocepham-4-carboxylic acid
(note the new numbering for cepham; it is different than that reported in ref. 9)

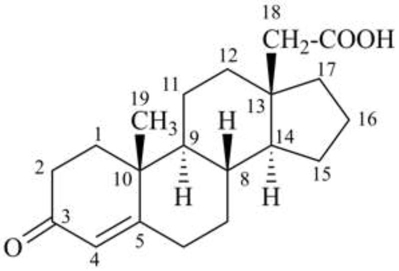
P-101.7.1.3 Substitution on terminal segments

Substitution on terminal segments by prefixes and suffixes expressing characteristic groups is recommended, even when a carbon atom included in a characteristic group is present. Lengthening a terminal segment by two methylene groups is allowed and is denoted by the use of the prefix 'dihomo'. Further lengthening is possible, but alkyl groups must be used, as an exception to the rule related to seniority of the longest chain.

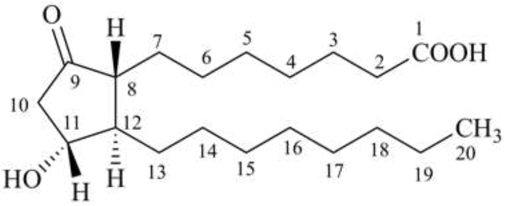
Examples:



3-oxoandrost-4-en-18-oic acid



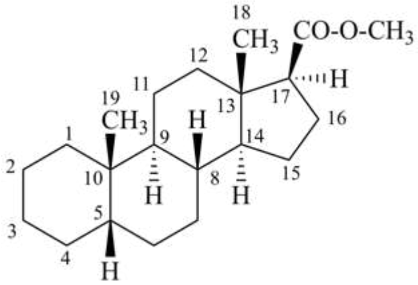
3-oxoandrost-4-ene-18-carboxylic acid



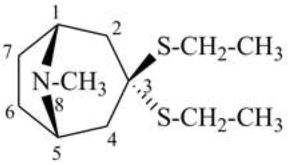
11α-hydroxy-9-oxoprostan-1-oic acid

P-101.7.2 Modifications to principal characteristic groups such as esters (see P-65.6.3.2), acetals (see P-66.6.5), etc. are named by the usual methods described in Chapter P-6. Cyclic modifications, such as lactones, cyclic acetals, etc. are named preferably as such rather than as fused or spiro ring systems, even if these names are functional class names (see also P-101.7.4).

Examples:



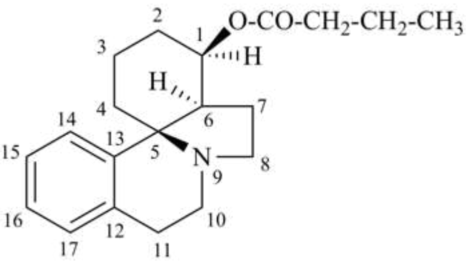
methyl 5β-androstane-17β-carboxylate



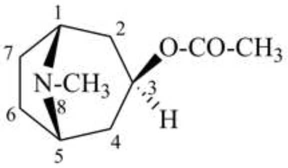
(1*R*,5*S*)-3,3-bis(ethylsulfanyl)-8-methyl-8-azabicyclo[3.2.1]octane
3,3-bis(ethylsulfanyl)tropane
tropan-3-one diethyl dithioketal

P-101.7.3 Names of substituent groups derived from parent structures are formed, by the general method described in P-29, by adding the suffixes ‘yl’, ‘ylidene’, or ‘ylidyne’, as appropriate, to the name of a parent, with elision of the final letter ‘e’, if present, before the letter ‘y’.

Examples:



erythrinan-1β-yl butanoate

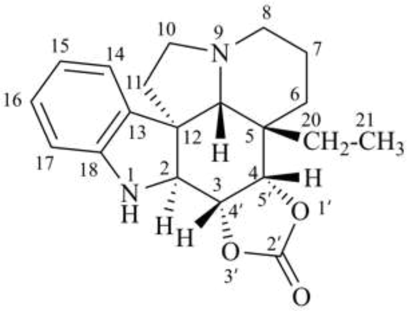


tropan-3β-yl acetate
(1*R*,3*s*,5*S*)-8-methyl-8-azabicyclo[3.2.1]octan-3-yl acetate
(see P-93.5.2.2.1)

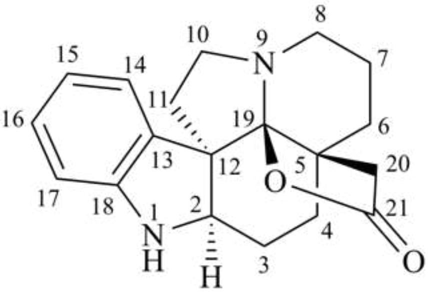
P-101.7.4 Addition of rings denoting functional groups

Rings denoting functional groups are preferably named by the usual methods described for constructing systematic names. Cyclic esters and lactones are named by the general method described for naming esters (see P-65.6.3.5). Names of acetals are formed by using the principles of functional class nomenclature (see P-66.6.5) rather than by fusion nomenclature described in P-101.5. When a choice is possible, a fusion name is preferred.

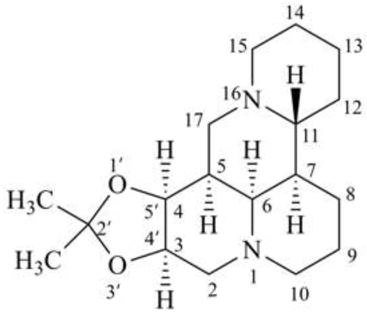
Examples:



(3β*H*,4β*H*)-3,4-dihydro[1,3]dioxolo[4′,5′:3,4]aspidospermidin-2′-one
aspidospermidine-3α,4α-diyl carbonate (see P-65.6.3.5.4)



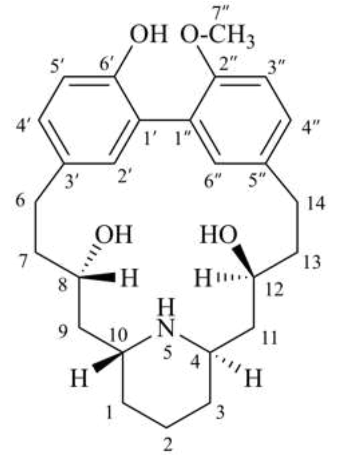
19,21-epoxyaspidospermidin-21-one
21-noraspidospermidine-20,19-carbolactone (see P-65.6.3.5.1)
19-hydroxyaspidospermidine-21,19-lactone

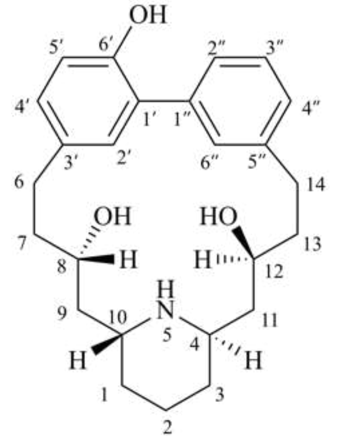


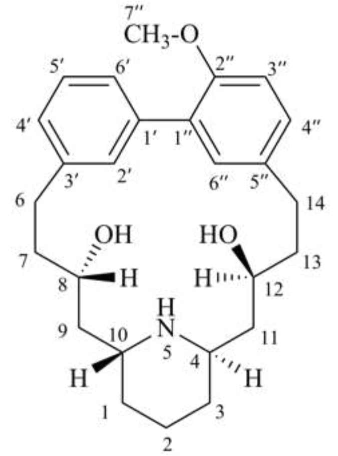
(3α*H*,4α*H*)-2′,2′-dimethyl-3,4-dihydro[1,3]dioxolo[4′,5′:3,4]matridine
propan-2-one matridine-3β,4β-diyl ketal (see P-66.6.5)
acetone matridine-3β,4β-diyl ketal

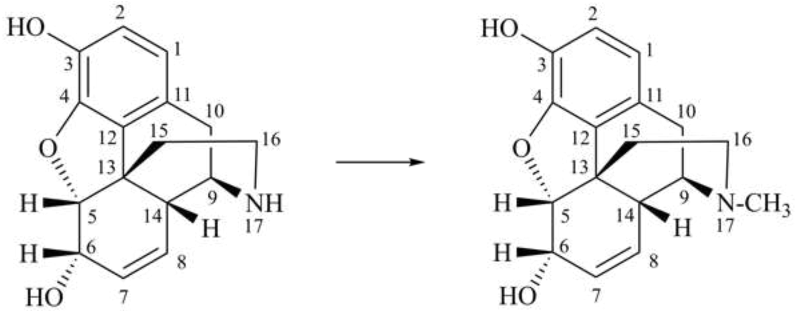
P-101.7.5 The prefix ‘de’ (not ‘des’), followed by the name of a group or atom (other than hydrogen), denotes removal of that group or atom and addition of hydrogen atoms as necessary. The prefix ‘de’ is currently used in carbohydrate nomenclature (see P-102.5.3) to indicate the removal of an oxygen atom from –OH with reconnection of the hydrogen atom.

Examples:


lythranidine
(fundamental parent structure)


2″-demethoxylythranidine


6′-deoxylythranidine



I **II**

morphine demethylmorphine

I (5β*H*)-17-methyl-7,8-didehydrofuro[2′,3′,4′,5′:4,12,13,5]morphinan-3,6α-diol
II (5β*H*)-7,8-didehydrofuro[2′,3′,4′,5′:4,12,13,5]morphinan-3,6α-diol

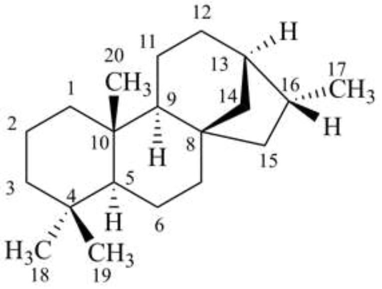
P-101.8 FURTHER ASPECTS OF CONFIGURATIONAL SPECIFICATION

In addition to the specification of the absolute configuration of fundamental and modified parent structures using ‘α’, ‘β’, ‘ξ’, ‘*R*’, and ‘*S*’ stereodescriptors, many other stereochemical features have to be described. The principles, rules and conventions described in Chapter P-9 are applied.

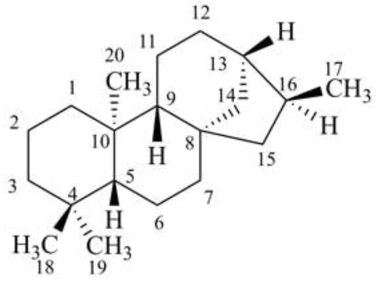
P-101.8.1 Inversion of configuration

Configurational inversion of all chirality centers is indicated by the italicized prefix ‘*ent*’ (a contracted form for ‘*enantio*’) placed at the front of the complete name of the compound. This prefix denotes inversion at all chirality centers (including those due to named substituents) whether these are cited separately or are implied in the name. For kaurane and *ent*-kaurane illustrated below, correct structures and names are given; the designations are reversed by Chemical Abstracts (see ref. 22).

Example:



kaurane



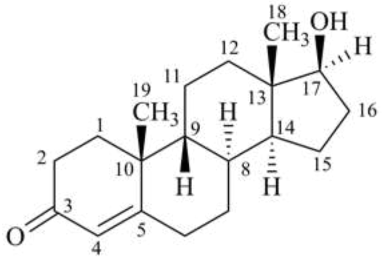
ent-kaurane

P-101.8.2 Racemates

Racemates are named by citing the italicized stereodescriptor ‘*rac*’ (an abbreviation for *racemo*) in front of the whole name of the compound including the prefix ‘*epi*’, if present. In the case of a racemic compound, the enantiomeric structure drawn should be the one that shows the lowest numbered chirality center in the α-configuration. This may differ from the usual practice, which is to draw the enantiomeric structure having the same absolute configuration as the naturally occurring substance.

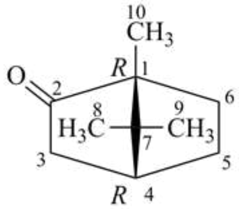
P-101.8.3 Relative configuration

When the relative, but not the absolute configurational relationships among chirality centers are known, the symbol ‘*rel*’ in association with *R* or *S* (preferred to ‘*R**’ and/or ‘*S**’) is used in accordance with Rule P-93.5.1.2. Alternatively, enantiomers of known relative, but unknown absolute, configuration may be distinguished by the compound stereodescriptor (+)-*rel*- or (–)-*rel*-, where the plus and minus sign refer to the direction of rotation of polarized light at the sodium D line. Hence, the dextrorotatory form of the following structure would be named (+)-*rel*-17β-hydroxy-8α,9β-androst-4-en-3-one.

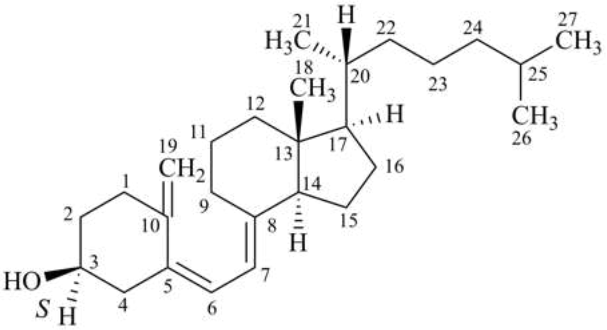


P-101.8.4 The stereodescriptors ‘*R*’ and ‘*S*’ are used to describe the absolute configuration of stereogenic centers for a compound whose parent structure is achiral, for example bornane. They are also used, in place of ‘α’, ‘β’, ‘ξ’, when a ring is opened creating two chiral portions, one of which may rotate, as shown for vitamin D.

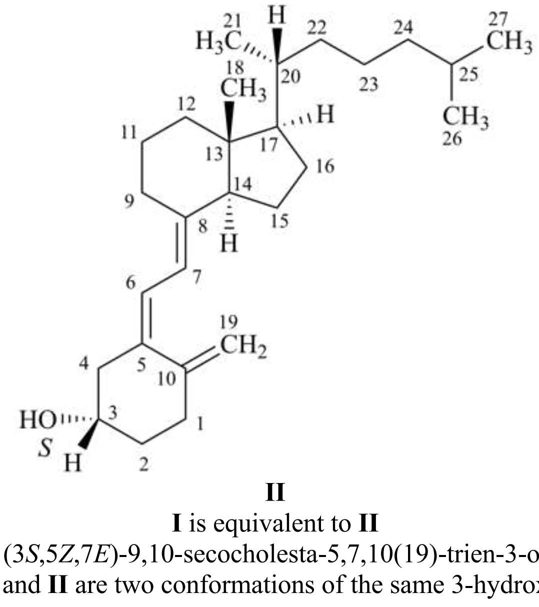
Example:



(1*R*,4*R*)-bornan-2-one
(+)-camphor
(1*R*,4*R*)-1,7,7-trimethylbicyclo[2.2.1]heptan-2-one



I



II
I is equivalent to **II**
(3*S*,5*Z*,7*E*)-9,10-secocholesta-5,7,10(19)-trien-3-ol
[structures **I** and **II** are two conformations of the same 3-hydroxy derivative]

P-102 CARBOHYDRATE NOMENCLATURE

P-102.0 INTRODUCTION

Nomenclature of carbohydrates is based on the concept of parent monosaccharides having retained names. These structures and names can be modified to indicate the nature of characteristic groups that are present, such as aldehydes, carboxylic acids, alcohols. They can also be combined to form di-, tri-, and oligosaccharides.

The nomenclature has been recently revised (ref. 27). This Section describes the basic concepts of this specific type of nomenclature, in particular the extensive system of symbols and stereodescriptors to indicate the configuration of the many diastereoisomers and enantiomers.

P-102.1 Definitions
P-102.2 Parent monosaccharides
P-102.3 Configurational symbolism
P-102.4 Choice of a parent structure
P-102.5 Monosaccharides: aldoses and ketoses; deoxy and amino sugars
P-102.6 Monosaccharides and derivatives as substituent groups
P-102.7 Disaccharides and oligosaccharides

P-102.1 DEFINITIONS

P-102.1.1 Carbohydrates
P-102.1.2 Monosaccharides
P-102.1.3 Oligosaccharides
P-102.1.4 Polysaccharides

P-102.1.1 Carbohydrates

The generic term ‘carbohydrates’ includes monosaccharides, oligosaccharides, and polysaccharides as well as substances derived from monosaccharides by reduction of the carbonyl group (alditols), by oxidation of one or more terminal groups to carboxylic acids, or by replacement of one or more hydroxy group(s) by a hydrogen atom, an amino group, a thiol group, or similar heteroatomic groups. It also includes derivatives of these compounds. The term ‘sugar’ is frequently applied to monosaccharides and lower oligosaccharides.

Cyclitols are generally not regarded as carbohydrates. For nomenclature of cyclitols, see P-104 and ref. 39.

P-102.1.2 Monosaccharides

Parent monosaccharides are polyhydroxy aldehydes H-[CHOH]$_n$-CHO or polyhydroxy ketones H-[CHOH]$_m$-CO-[CHOH]$_n$-H with three or more carbon atoms.

The generic term ‘monosaccharide’ (as opposed to oligosaccharide or polysaccharide) denotes a single unit without glycosidic connections to other such units and includes aldoses, dialdoses, aldoketoses, ketoses, diketoses, as well as deoxy sugars and amino sugars, and their derivatives, provided that the parent compound has a (potential) carbonyl group.

Names for monosaccharides are either trivial or systematic. Many trivial names such as glucose, fructose, etc. are retained and used to describe the corresponding functional parents. This aspect of carbohydrate nomenclature is limited because it applies only to monosaccharides having four to six carbon atoms. A ‘systematic carbohydrate nomenclature’ has been developed that is applicable to compounds with four or more carbon atoms, and is used extensively by carbohydrate chemists for compounds with more than six carbon atoms, and for unsaturated or branched sugars. In these recommendations, these names are called ‘systematic carbohydrate names’ to differentiate them from names formed systematically by applying principles, rules and conventions of substitutive nomenclature discussed in Chapters P-1 to P-9 of these Recommendations that are called ‘substitutive names’ or ‘systematic substitutive names’ (see P-102.5.2.3 for a discussion on and the illustration of these two types of nomenclature).

P-102.1.2.1 Aldoses and ketoses

Monosaccharides with an aldehydic carbonyl or potential aldehydic carbonyl group are called aldoses; those with a ketonic carbonyl or potential carbonyl group, ketoses.

Addition of a numerical prefix (e.g. ‘pent’, ‘hex’) indicates the number of carbon atoms present (e.g. ‘aldopentose’, ‘ketohexose’).

The term ‘potential aldehydic group’ refers to the hemiacetal group arising from ring closure; the term ‘potential ketonic group’ refers to the hemiketal structure.

Cyclic hemiacetals or hemiketals of sugars with a five-membered ring (oxolane or tetrahydrofuran) ring are called ‘furanoses’, those with a six-membered ring (oxane or tetrahydropyran) ring ‘pyranoses’.

Dialdoses are monosaccharides containing two (potential) aldehydic groups.

Diketoses are monosaccharides containing two (potential) ketonic groups.

Ketoaldoses are monosaccharides containing one (potential) aldehydic group and one (potential) ketonic group; this term is preferred to ‘aldoketoses’ and ‘aldosuloses’.

P-102.1.2.2 Deoxysugars

Monosaccharides in which an alcoholic hydroxy group has been replaced by a hydrogen atom are called ‘deoxy sugars’.

P-102.1.2.3 Amino sugars

Monosaccharides in which an alcoholic hydroxy group has been replaced by an amino group are called ‘amino sugars’. When the hemiacetal group is replaced by an amino group, the compounds are called ‘glycosylamines’.

P-102.1.2.4 Glycosides

Glycosides are mixed acetals formally arising by elimination of water between the hemiacetal or hemiketal hydroxy group of a sugar and a hydroxy group of a second compound. The bond between the two components is called a ‘glycosidic bond’.

P-102.1.3 Oligosaccharides

Oligosaccharides are compounds in which monosaccharide units are joined by glycosidic linkages. According to the number of units, they are called disaccharides, trisaccharides, etc. The maximum number of units is not defined.

P-102.1.4 Polysaccharides

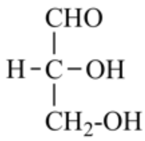
‘Polysaccharide’ (glycan) is the name given to a macromolecule consisting of a large number of monosaccharide (glycose) residues joined to each other by glycosidic linkages. The term ‘poly(glycose)’ is not a synonym for polysaccharide (glycan), because it includes monosaccharide residues joined to each other by nonglycosidic linkages.

P-102.2 PARENT MONOSACCHARIDES

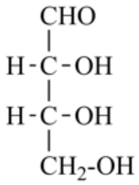
P-102.2.1 The bases for carbohydrate names are the structures of the parent monosaccharides in their acyclic form. Tables 10.2 and 10.3 give retained names for parent aldoses and ketoses with up to six carbon atoms. These retained names are customarily used when the acyclic aldose or ketose has a carbon chain consisting of four, five, or six carbon atoms. Names of monosaccharides whose carbon skeleton is composed of more than six carbon atoms are systematic carbohydrate names.

In Table 10.2 structures and retained names of the aldoses (in the aldehydic, acyclic form) with three through six carbon atoms are described. Only the D-forms are shown; the L-forms are the mirror images.

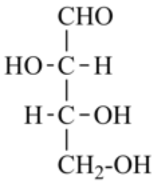
Table 10.2 Retained and systematic carbohydrate names and structures (in the aldehydic acyclic form) of the aldoses with three through six carbon atoms



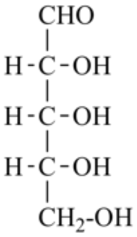
(2*R*)-2,3-dihydroxypropanal
D-glyceraldehyde
D-*glycero*-triose



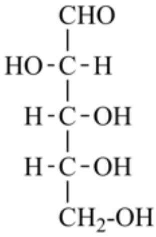
D-erythrose
D-*erythro*-tetrose



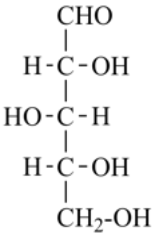
D-threose
D-*threo*-tetrose



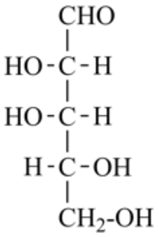
D-ribose
D-*ribo*-pentose



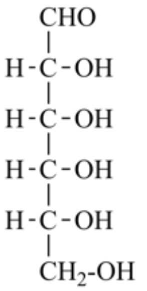
D-arabinose
D-*arabino*-pentose

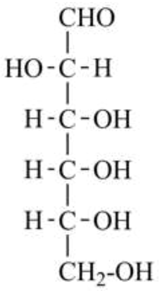


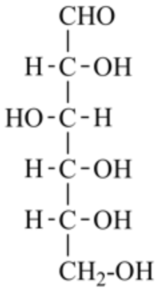
D-xylose
D-*xylo*-pentose

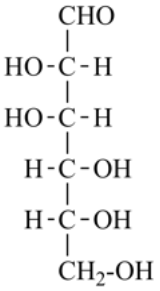


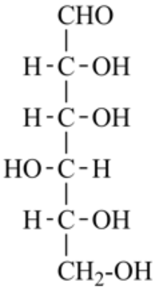
D-lyxose
D-*lyxo*-pentose

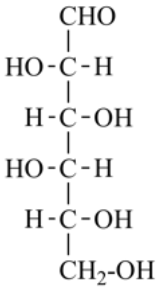

D-allose
D-*allo-hexose*

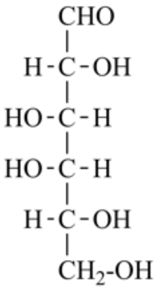

D-altrose
D-*altro*-hexose

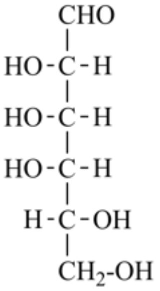

D-glucose
D-*gluco*-hexose


D-mannose
D-*manno*-hexose


D-gulose
D-*gulo*-hexose

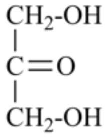

D-idose
D-*ido*-hexose

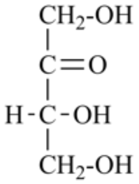

D-galactose
D-*galacto*-hexose

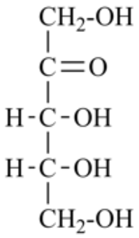

D-talose
D-*talo*-hexose

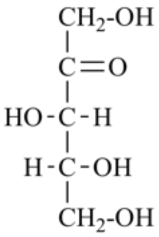
In Table 10.3 structures and retained names of the 2-ketoses (in the ketonic, acyclic form) with three through six carbon atoms are described. Only the D-forms are shown; the L-forms are the mirror images.

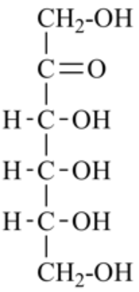
Table 10.3 Structures, and carbohydrate names, of the 2-ketoses with three through six carbon atoms

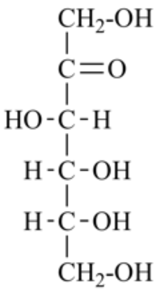

1,3-dihydroxypropan-2-one
1,3-dihydroxyacetone
glycerone

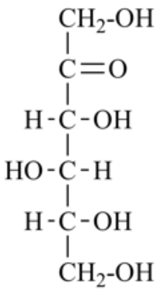

D-erythrulose

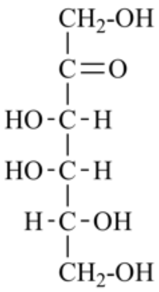

D-ribulose


D-xylulose


D-psicose
D-*ribo*-hex-2-ulose


D-fructose
D-*arabino*-hex-2-ulose


D-sorbose
D-*xylo*-hex-2-ulose


D-tagatose
D-*lyxo*-hex-2-ulose

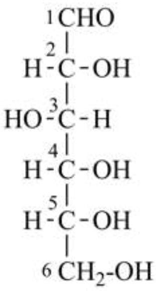
P-102.2.2 Numbering parent structures

The carbon atoms of a monosaccharide are numbered consecutively in such a way that:

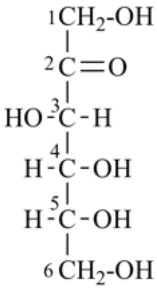
(1) a (potential) aldehyde group receives the locant 1 (even if a more senior characteristic group is present);

(2) the most senior of other characteristic groups expressed in the suffix receives the lowest possible locant, i.e carboxylic acid (derivatives) > (potential) ketonic carbonyl groups.

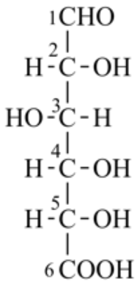
Examples:



D-glucose



D-fructose

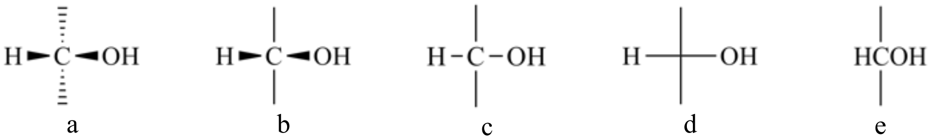


D-glucuronic acid

P-102.3 CONFIGURATIONAL SYMBOLISM

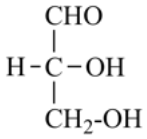
P-102.3.1 The Fischer projection of the acyclic form

In this representation of a monosaccharide, the carbon chain is written vertically with the lowest numbered carbon at the top, as indicated in P-102.2.2. To define the configuration, each carbon atom is considered in turn and placed in the plane of the paper. Neighboring carbon atoms are below, and the H atoms and OH groups are above the plane of the paper. Various representations 'b', 'c', 'd', 'e' and 'f' of a carbon atom in a monosaccharide in the Fischer projection are as follows (structure 'a' is a three-dimensional representation; the real Fischer projection is 'd'). The representation 'c' is commonly used in these recommendations.

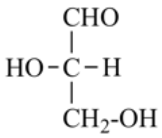


P-102.3.2 The stereodescriptors 'D' and 'L'

The simplest aldose is glyceraldehyde. It contains one center of chirality and occurs therefore in two enantiomeric forms, called D-glyceraldehyde and L-glyceraldehyde; these are represented by the Fischer projection formulas given below. It is known that these projections correspond to the absolute configurations. The configurational stereodescriptors 'D' and 'L' must be written in small capital letters and linked by a hyphen to the name of the sugar. The configuration is often described by the preferred CIP stereodescriptors *R* and *S*.



D-glyceraldehyde
(2*R*)-2,3-dihydroxypropanal

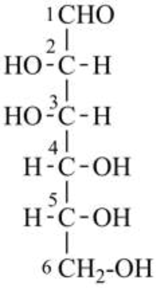


L-glyceraldehyde
(2*S*)-2,3-dihydroxypropanal

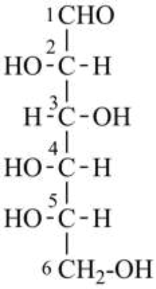
P-102.3.3 The configurational atom

A monosaccharide is assigned to the ‘D’ or ‘L’ series according to the configuration of the highest numbered chirality center. This asymmetrically substituted carbon atom is called the ‘configurational atom’. Thus if the hydroxy group projects to the right in the Fischer projection, the sugar belongs to the ‘D’ series, and receives the ‘D’ stereodescriptor.

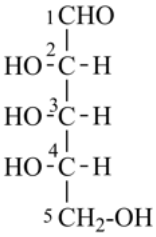
Examples:



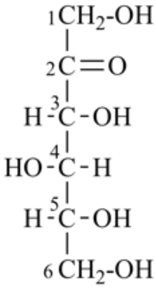
D-mannose



L-glucose



L-ribose



D-sorbose

P-102.3.4 Cyclic forms of monosaccharides

Most monosaccharides exist as cyclic hemiacetals or hemiketals. Two aspects of the internal cyclisation must be examined: first, the size of the ring, and secondly, the configuration of the newly created chirality center.

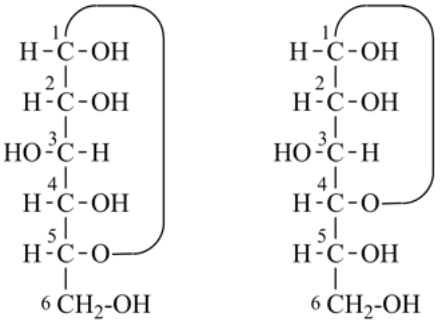
P-102.3.4.1 Ring size

Out of the various possible heterocyclic ring sizes resulting from hemiacetal or hemiketal formation, those with five and six members, including an oxygen atom, prevail and are discussed in this Section. Their names are based on those of the parent heterocycles furan and pyran, respectively. Names are formed by including the terms ‘furan’ and ‘pyran’ before the ending 'ose' in the name of a sugar. For example, D-mannose is changed to D-mannopyranose to indicate the cyclic form having a six-membered ring; furthermore, the generic term 'pyranose' includes all the sugars having a six-membered ring structure. Similarly, the sugars having a five-membered ring structure are 'furanoses'; oxiroses, oxetoses and septanoses have a three-, four- or seven-membered cyclic structure, respectively.

Different representations of cyclic forms are to be considered.

P-102.3.4.1.1 Hemiacetal or hemiketal formation is indicated in the Fischer projection of the cyclic form by a long bond joining the original aldehydic or ketonic group to the oxygen atom included in the ring.

Examples:



D-glucopyranose D-glucofuranose

P-102.3.4.1.2 The Haworth representation

The Haworth representation is a perspective drawing. The ring is orientated almost perpendicular to the plane of the paper, but viewed from slightly above so that the edge closer to the viewer is drawn below the most distant edge, with the oxygen behind and 'C-1' at the right hand end. The cyclisation process is envisaged as proceeding stepwise, as exemplified for D-glucopyranose in Fig. 10.1.

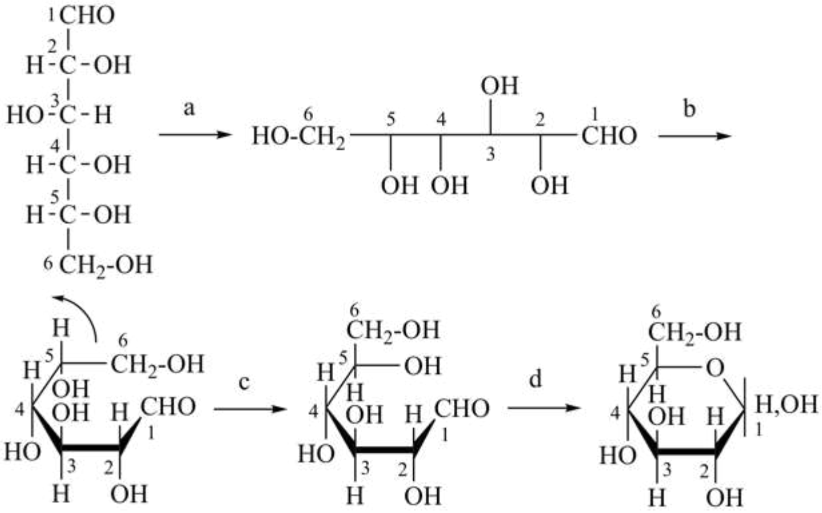


Fig. 10.1 Reorientation of a Fischer projection to a Haworth projection

Two reorientations are necessary from the standard Fischer projection to prepare the acetalization or ketalization procedure: the first reorientation, step (a), consists in placing the nonterminal hydroxy groups vertically; the second reorientation, step (c), is the rotation at carbon C-5 to place the oxygen atom in the plane of the ring. The structure is defined completely by expressing the configuration at carbon '1'.

P-102.3.4.2 Anomeric forms; the stereodescriptors 'α' and 'β'

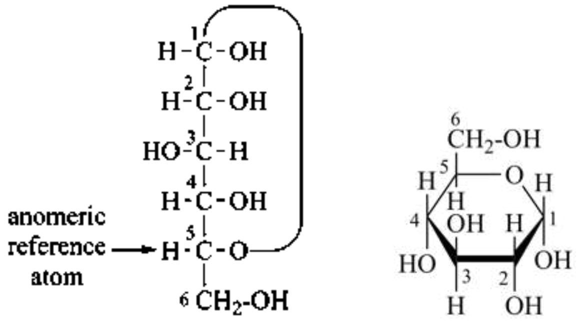
P-102.3.4.2.1 In the cyclic form, the configuration of the newly created chirality center 'C-1' must be expressed. This center is called the 'anomeric center'. The two stereoisomers are called 'anomers'; they are designated by the stereodescriptors 'α' and 'β' according to the configurational relationship between the anomeric center and the so called 'reference center'.

P-102.3.4.2.2 Configurations 'α' and 'β' for monosaccharides

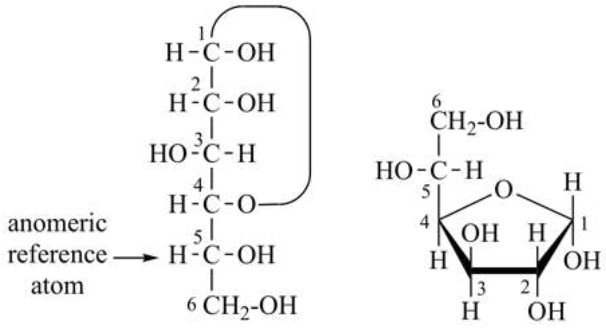
The anomeric reference center in a monosaccharide having a retained name is the configurational atom as defined in P-102.3.3. In the Fischer projection, the α-anomer has the exocyclic oxygen atom at the anomeric center formally '*cis*' to the oxygen atom attached to the anomeric reference atom; in the β-anomer, the relationship is '*trans*'. The reference plane for determining the configurations '*cis*' and '*trans*' is perpendicular to the Fischer projection, including all carbon atoms of the monosaccharide.

The anomeric stereodescriptor 'α' or 'β', followed by a hyphen, is placed immediately before the configurational stereodescriptor 'D' or 'L' of the carbohydrate name.

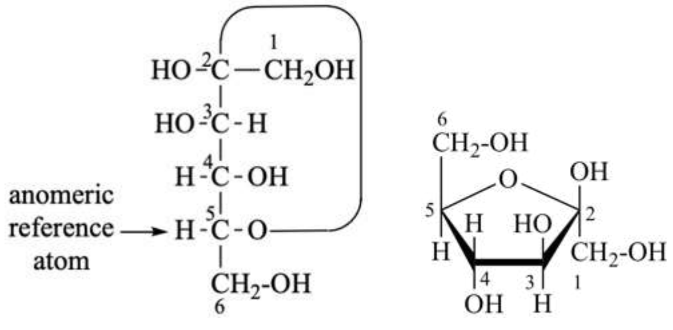
Examples:



α-D-glucopyranose



α-D-glucofuranose

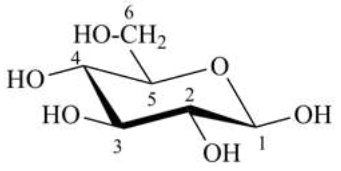


β-D-fructofuranose

P-102.3.5 Conformation of monosaccharides

Pyranoses assume conformations that are not planar. For example β-D-glucopyranose assumes a chair conformation with characteristic substituent groups in equatorial conformations (hydrogen atoms attached to the ring are not shown):

Example:

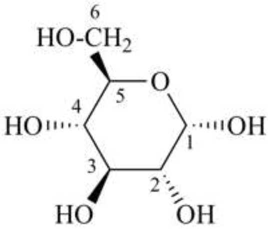


β-D-glucopyranose

P-102.3.6 The Mills depiction

In this depiction, the main hemiacetal ring is drawn in the plane of the paper. Hashed wedges denote substituents below this plane, and solid wedges those above.

Example:



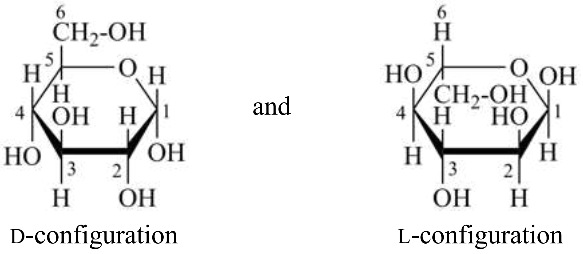
α-D-glucopyranose

P-102.3.7 Stereodescriptors for denoting racemates and uncertain configurations

P-102.3.7.1 Stereodescriptors for denoting racemates

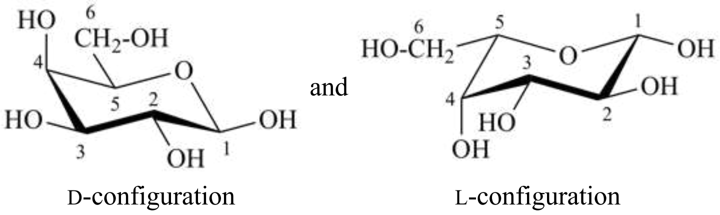
Racemates are indicated by the stereodescriptor 'DL'.

Examples:



D-configuration L-configuration

α-DL-glucopyranose



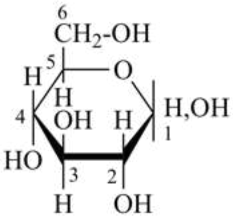
D-configuration L-configuration

β-DL-galactopyranose

P-102.3.7.2 Mixtures of anomers

When a mixture of anomers has to be described, the stereodescriptors 'α' and 'β' are placed at the front of the name, separated by a comma; in Haworth representations, the symbols H and OH replace the formal bonds at the anomeric carbon atom.

Example:



α,β-D-glucopyranose

P-102.4 CHOICE OF PARENT STRUCTURE

In cases where more than one monosaccharide structure is embedded in a large molecule, a parent structure is chosen on the basis of the following criteria, applied in the order given until a decision is reached:

(a) the parent that includes the functional group most senior in the order of classes (see P-41). If there is a choice, it is made on the basis of the greatest number of occurrences of the most senior functional group.

Thus, ketoaldaric acid/aldaric acid > ketouronic acid/uronic and ketoaldonic acid/aldonic acid > dialdose > ketoaldose/aldose > diketose > ketose;

(b) the parent with the greatest number of carbon atoms in the chain, for example, heptose rather than hexose;

(c) the parent with the name that comes first in an alphabetical listing based on the following:

(i) the trivial name or the configurational prefix(es) of the systematic name, for example, glucose rather than gulose; a gluco rather than a gulo derivative;

Example: D-glucitol; not L-gulitol (see P-102.5.6.5.1);

(ii) the configurational symbol D rather than L;

Example: 5-*O*-methyl-D-galactitol; not 2-*O*-methyl-L-galactitol (see P-102.5.6.5.2);

(iii) the anomeric stereodescriptor α rather than β;

Example: α-D-fructofuranose β-D-fructofuranose 1,2′:1′,2-dianhydride; not β-D-fructofuranose α-D-fructofuranose 1,2′:1′,2-dianhydride (see P-102.5.6.7.2);

(d) the parent with the most substituent groups cited as prefixes (bridging substitution for example, 2,3-*O*-methylene is regarded as multiple substitution for this purpose); the prefixes ‘deoxy’ and ‘anhydro’ are detachable and alphabetized, thus regarded as substituent groups;

(e) the parent with the lowest locants for substituent prefixes;

Example: 2,3,5-tri-*O*-methyl-D-mannitol; not 2,4,5-tri-*O*-methyl-D-mannitol [see P-102.5.6.5.3 (a)]

(f) the parent with the lowest locant for the first cited substituent.

Example: 2-*O*-acetyl-5-*O*-methyl-D-mannitol; not 5-*O*-acetyl-2-*O*-methyl-D-mannitol [see P-102.5.6.5.3 (b)].

P-102.5 MONOSACCHARIDES: ALDOSES AND KETOSES; DEOXY AND AMINO SUGARS

P-102.5.1 Aldoses
P-102.5.2 Ketoses
P-102.5.3 Deoxy sugars
P-102.5.4 Amino sugars
P-102.5.5 Thio sugars
P-102.5.6 Substituted monosaccharides

P-102.5.1 Aldoses

Names of aldoses are retained or substitutively formed. Retained and semisystematic carbohydrate names for aldoses with three through six carbon atoms are listed in Table 10.2.

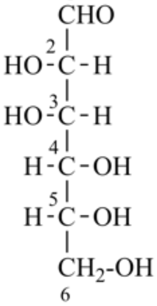
Names of aldoses having more than six carbon atoms are formed in two ways: by the procedures of systematic carbohydrate nomenclature, and by those of systematic substitutive nomenclature.

P-102.5.1.1 Systematic carbohydrate names

Systematic carbohydrate names of aldoses are formed from a stem name and a configurational prefix or prefixes. Stem names for the aldoses with three through ten carbon atoms are triose, tetrose, pentose, hexose, heptose, octose, nonose, and decose. The chain is numbered so that the carbonyl group receives the locant ‘1’.

P-102.5.1.1.1 The configuration of >CH-OH groups of the sugar is designated by the configurational prefix(es) listed in Table 10.2, such as ‘*glycero*’, ‘*gluco*’, ‘*manno*’, etc. Each name is qualified by a ‘D’ or ‘L’ stereodescriptor, as defined in P-102.3.2.

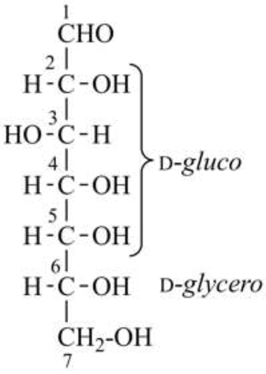
Example:



D-*manno*-hexose (systematic carbohydrate name)
D-mannose (retained name)

P-102.5.1.1.2 Aldoses composed of more than four chirality centers are named by adding two or more configurational prefixes (listed in Table 10.2) to the stem name. Prefixes are assigned in order to the chirality centers in groups of four, beginning with the group located next to the aldehydic group. The prefix relating to the group of carbon atoms farthest from the aldehydic group (which may contain fewer than four chirality centers) is cited first.

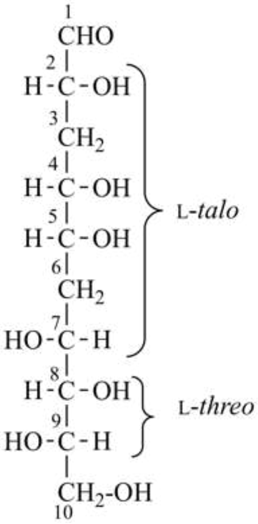
Example:



D-*glycero*-D-*gluco*-heptose
(not D-*gluco*-D-*glycero*-heptose)
(2*R*,3*S*,4*R*,5*R*,6*R*)-2,3,4,5,6,7-hexahydroxyheptanal

P-102.5.1.1.3 When sequences of chirality centers are separated by nonchiral centers, the nonchiral centers are ignored, and the remaining set of chirality centers is assigned the appropriate configurational prefix (for four centers or less) or prefixes (for more than four centers).

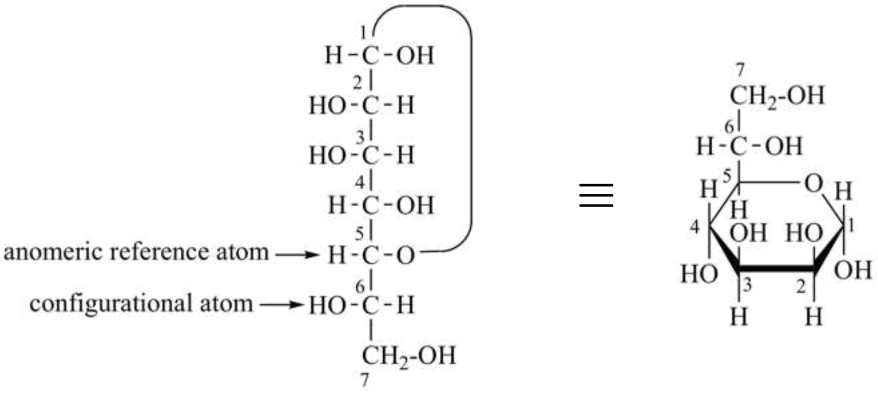
Example:



3,6-dideoxy-L-*threo*-L-*talo*-decose
(for deoxy sugars, see P-102.5.3)
(2*R*,4*S*,5*R*,7*R*,8*S*,9*S*)-2,4,5,7,8,9,10-heptahydroxydecanal

P-102.5.1.1.4 Cyclic forms

For monosaccharides having more than six carbon atoms, the anomeric reference center is the highest numbered atom of the group of chirality centers next to the anomeric center that is involved in the heterocyclic ring and specified by a single configurational prefix. In the α-anomer, the exocyclic oxygen atom at the anomeric center is formally '*cis*', in the Fischer projection, to the oxygen atom attached to the anomeric reference atom; in the β-anomer these oxygen atoms are formally '*trans*'.



L-*glycero*-α-D-*manno*-heptopyranose
(2*S*,3*S*,4*S*,5*S*,6*R*)-6-[(1*S*)-1,2-dihydroxyethyl]oxane-2,3,4,5-tetrol

P-102.5.2 Ketoses

P-102.5.2.1 Classification

Ketoses are classified as 2-ketoses, 3-ketoses, etc. according to the lowest locant for the position of the (potential) carbonyl group.

P-102.5.2.2 Retained names

Retained names and structures are shown in Table 10.3; the configuration is specified by a ‘D’ or ‘L’ stereodescriptor, as defined in P-102.3.2.

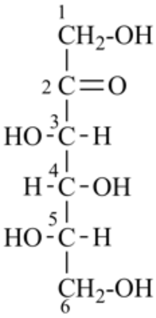
P-102.5.2.3 Systematic carbohydrate names

The systematic carbohydrate names of ketoses having four through six carbon atoms are formed from the stem name and the appropriate configurational prefix listed in Table 10.3. The stem names are formed from the corresponding aldoses stem names by replacing the ending ‘ose’ with ‘ulose’, preceded by the locant of the carbonyl group, e.g. ‘pent-2-ulose’ and ‘hex-3-ulose’. The chain is numbered so that the carbonyl group receives the lowest possible locant. When the carbonyl group is in the middle of a chain with an odd number of carbon atoms, a choice between alternative names is made according to P-102.4.

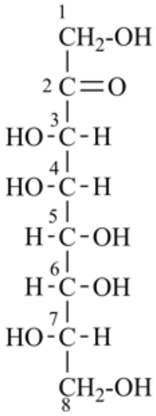
For 2-ketoses, configurational prefixes are given in the same way as for aldoses.

Substitutive names are given after the ‘systematic carbohydrate names’ to illustrate the two types of systematic names that are recommended in carbohydrate nomenclature.

Examples:



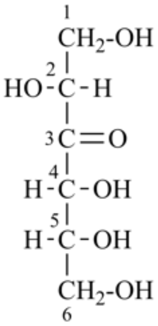
L-*xylo*-hex-2-ulose
L-sorbose



L-*glycero*-D-*manno*-oct-2-ulose
(3*S*,4*S*,5*R*,6*R*,7*S*)-1,3,4,5,6,7,8-heptahydroxyoctan-2-one

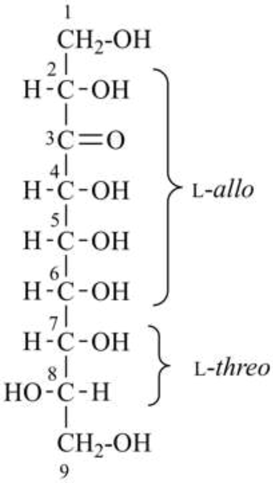
For ketoses with the carbonyl group at C-3, or at a higher-numbered carbon atom, the carbonyl group is ignored and the set of chirality centers is given the appropriate prefix or prefixes according to Table 10.3.

Examples:



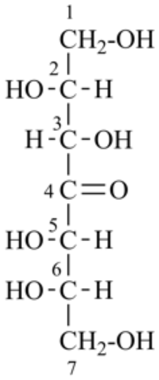
D-*arabino*-hex-3-ulose

(2*R*,4*R*,5*R*)-1,2,4,5,6-pentahydroxyhexan-3-one

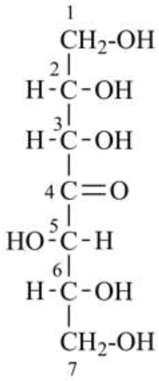


L-*threo*-D-*allo*-non-3-ulose

(2*S*,4*R*,5*R*,6*R*,7*R*,8*S*)-1,2,4,5,6,7,8,9-octahydroxynonan-3-one



not



L-*gluco*-hept-4-ulose

[not D-*gulo*-hept-4-ulose;

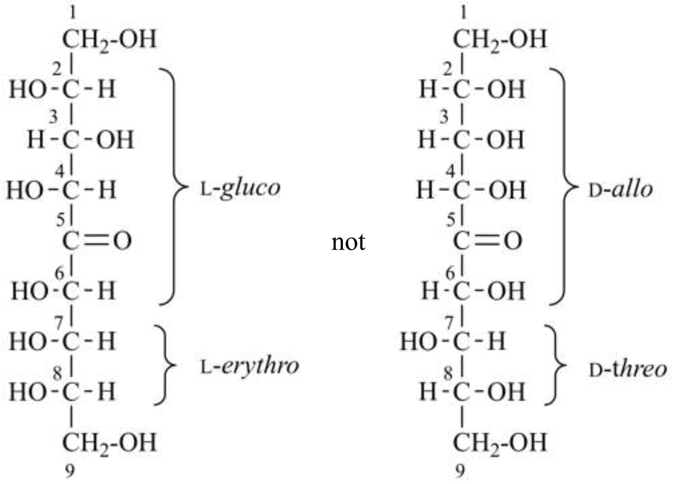
gluco is earlier in alphanumerical order, see P-102.4 (c)]

(2*R*,3*S*,5*S*,6*S*)-1,2,3,5,6,7-hexahydroxyheptan-4-one

[not (2*S*,3*S*,5*S*,6*R*)-1,2,3,5,6,7-hexahydroxyheptan-4-one;

when there is a choice, the *R* configuration

is assigned the lowest locant, see P-14.4 (j)]



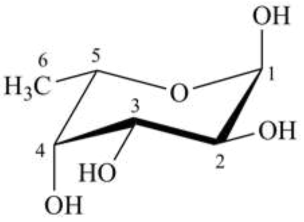
L-*erythro*-L-*gluco*-non-5-ulose
[not D-*threo*-D-*allo*-non-5-ulose;
erythro-*gluco* is earlier in alphanumerical order]
(2*R*,3*S*,4*R*,6*S*,7*S*,8*S*)-1,2,3,4,6,7,8,9-octahydroxynonan-5-one

P-102.5.3 Deoxy sugars

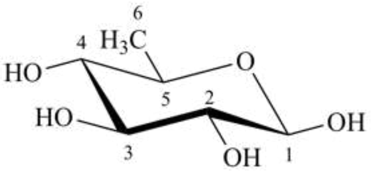
P-102.5.3.1 The prefix 'deoxy' describes the removal of an 'oxy' group, –O–, with rejoining of the hydrogen atom. In these recommendations, the prefix 'deoxy' is classified as detachable; i.e., it is alphabetized among the substituents arising from substitutive nomenclature. This is a change from the previous status (see R-0.1.8.4, ref. 2) that classified the prefix 'deoxy' among nondetachable prefixes (see also the prefix 'anhydro which is now classified as detachable and alphabetized among all detachable prefixes).

P-102.5.3.2 Trivial names.

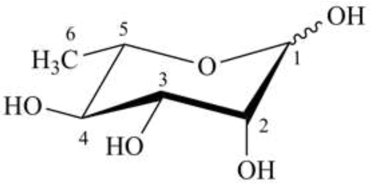
The following names are retained: fucose, quinovose and rhamnose. The corresponding structures are shown in the pyranose form.



α-L-fucopyranose
6-deoxy-α-L-galactopyranose



β-D-quinovopyranose
6-deoxy-β-D-glucopyranose



L-rhamnopyranose
6-deoxy-L-mannopyranose

P-102.5.3.3 Carbohydrate names derived from retained names

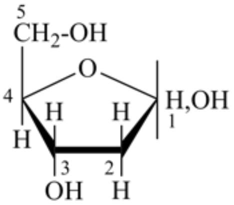
The prefix 'deoxy' is used in combination with a retained name when the deoxygenation does not involve the configuration at any chirality center, for example, 6-deoxy-D-allose. However the 6-deoxy derivatives of glucose, mannose, and galactose have their own retained trivial names (see P-102.5.3.2). When the prefix 'deoxy' modifies a chirality center, a carbohydrate name is preferred: names formed by substitutive nomenclature with CIP stereodescriptors are appropriate (see P-102.5.3.4 for examples).

The combination of ‘amino’ and ‘deoxy’ at the same position (and also the prefixes always cited as prefixes in substitutive nomenclature described in P-59.1.9 and ‘deoxy’ at the same position) is allowed.

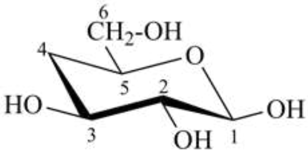
P-102.5.3.4 Systematic carbohydrate names

The systematic carbohydrate name consists of the prefix ‘deoxy’, preceded by the appropriate locant and followed by the stem name with such configurational prefixes as necessary to describe the chirality centers present in the deoxy compound. Configurational prefixes are cited in order commencing at the end furthest from C-1. The use of the prefix ‘deoxy’ with retained names of aldoses and ketoses is not recommended.

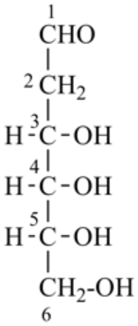
Examples:



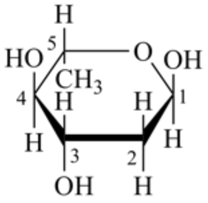
2-deoxy-D-*erythro*-pentofuranose
(often referred to as 2-deoxy-D-ribofuranose
or 2-deoxy-D-ribose)
(2ξ,4*S*,5*R*)-5-(hydroxymethyl)oxolane-2,4-diol



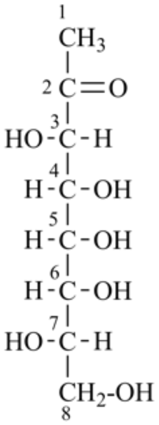
4-deoxy-β-D-*xylo*-hexopyranose
(not 4-deoxy-β-D-galactopyranose)
(2*R*,3*R*,4*S*,6*S*)-6-(hydroxymethyl)oxane-2,3,4-triol



2-deoxy-D-*ribo*-hexose (not 2-deoxy-D-allose)
(3*S*,4*S*,5*R*)-3,4,5,6-tetrahydroxyhexanal



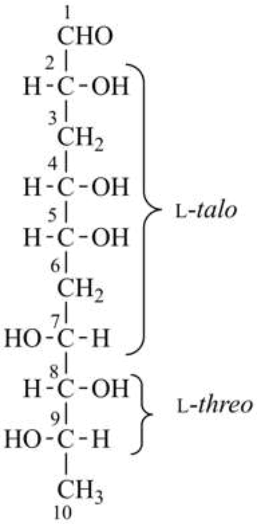
2,6-dideoxy-α-L-*arabino*-hexopyranose
(2*R*,4*S*,5*R*,6*S*)-6-methyloxane-2,4,5-triol



1-deoxy-L-*glycero*-D-*altro*-oct-2-ulose
(3*S*,4*R*,5*R*,6*R*,7*S*)-3,4,5,6,7,8-hexahydroxyoctan-2-one

When the –CH2– group divides the chirality centers into two sets, it is ignored for the purpose of assigning the configurational prefix; the prefix(es) assigned should cover the entire sequence of chirality centers (see aldoses) (see P-102.5.1.1.3).

Example:



3,6,10-trideoxy-L-*threo*-L-*talo*-decose
(2*R*,4*S*,5*R*,7*R*,8*R*,9*S*)-2,4,5,7,8,9-hexahydroxydecanal

P-102.5.4 Amino sugars

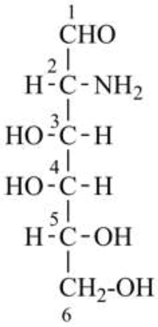
The replacement of a hydroxy group that is not an anomeric hydroxy group of a monosaccharide or a monosaccharide derivative by an amino group is envisaged as substitution of the appropriate hydrogen atom of the corresponding deoxy monosaccharide by an amino group. The configuration at the carbon atom carrying the amino group is expressed as that of an aldose, considering that the amino group has replaced a hydroxy group.

To the contrary, the replacement of a hydroxy group by a sulfanyl group is considered to be a functional replacement indicated by the prefix ‘thio’.

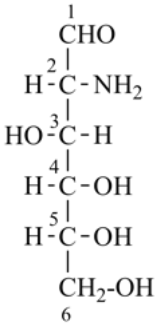
P-102.5.4.1 Amino sugars

P-102.5.4.1.1 Trivial names

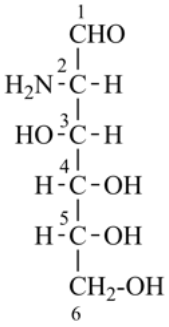
The following glycosamine names are retained.



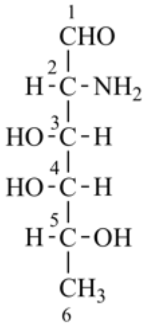
D-galactosamine
2-amino-2-deoxy-D-galactose



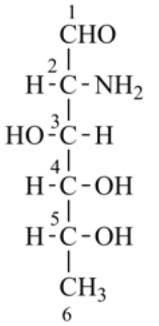
D-glucosamine
2-amino-2-deoxy-D-glucose



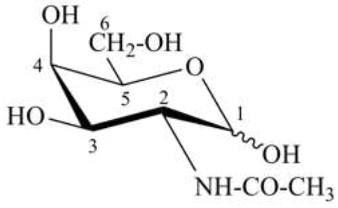
D-mannosamine
2-amino-2-deoxy-D-mannose



D-fucosamine
2-amino-2,6-dideoxy-D-galactose



D-quinovosamine
2-amino-2,6-dideoxy-D-glucose

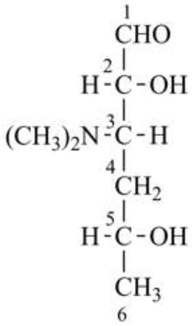


N-acetyl-D-galactosamine
2-acetamido-2-deoxy-D-galactopyranose

P-102.5.4.1.2 Systematic carbohydrate names

Systematic carbohydrate names are formed, in two steps: in a first step a deoxy sugar is created by deoxygenation at the carbon atom where the amino group is to be introduced by substitution in a second step. Names of substituted amines are formed by using the name of the substituted amino group as a prefix.

Example:



3,4,6-trideoxy-3-(dimethylamino)-D-*xylo*-hexose
(2*R*,3*S*,5*R*)-3-(dimethylamino)-2,5-dihydroxyhexanal

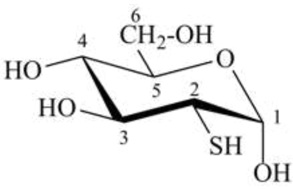
P-102.5.5 Thio sugars and other chalcogen analogues

The replacement of a hydroxy oxygen atom of an aldose or ketose, or of the oxygen atom of the carbonyl group of an acyclic aldose or ketose, by sulfur, selenium or tellurium is indicated by placing the prefix 'thio', 'seleno' or 'telluro', respectively, preceded by the appropriate locant, at the front of the systematic or trivial name of the aldose or ketose. In carbohydrate nomenclature, the prefixes 'thio', 'seleno' and 'telluro' are considered as detachable, alphabetized prefixes.

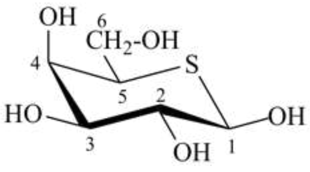
Replacement of the ring oxygen atom of the cyclic form of an aldose or ketose by sulfur, selenium, or tellurium is indicated in the same way, the number of the non-anomeric adjacent carbon atom of the ring being used as locant. In such a case, skeletal replacement expressed by an 'a' replacement prefix is not recommended.

Sulfoxides (and selenoxides or telluroxides) and sulfones (and selenones or tellurones) are named by functional class nomenclature (see P-63.6 for functional class names of sulfoxides and sulfones).

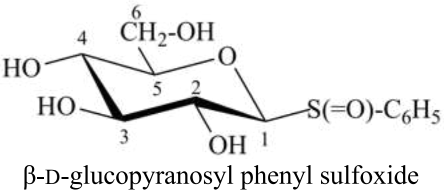
Examples:



2-thio-α-D-glucopyranose



5-thio-β-D-galactopyranose



β-D-glucopyranosyl phenyl sulfoxide
(for glycosyl groups, see P-102.6.1.1)
(2*S*,3*R*,4*S*,5*S*,6*R*)-2-(benzenesulfinyl)-6-(hydroxymethyl)oxane-3,4,5-triol

P-102.5.6 Monosaccharide derivatives

P-102.5.6.1 *O*-Substitution
P-102.5.6.2 Glycosides
P-102.5.6.3 *C*-Substitution
P-102.5.6.4 *N*-Substitution
P-102.5.6.5 Alditols
P-102.5.6.6 Monosaccharide carboxylic acids
P-102.5.6.7 Anhydrides

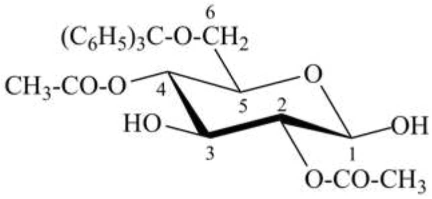
P-102.5.6.1 *O*-Substitution

In order to maintain the integrity of structures and take advantage of retained names to imply the absolute configuration, *O*-substitution is allowed in carbohydrate nomenclature. Substituents replacing the hydrogen atom of an alcoholic hydroxy group of a monosaccharide or monosaccharide derivative are denoted as *O*-substituents. The substitution of an anomeric hydroxy group is discussed in P-102.5.6.3.2. The *O*-locant is not repeated for multiple substitution by the same atom or group. Number locants are used as necessary to specify the positions of substituents; they are not required for compounds fully substituted by identical atoms or groups.

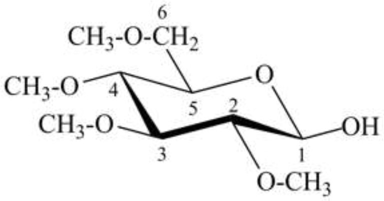
P-102.5.6.1.1 *O*-Acetyl and *O*-alkyl functionalization.

For *O*-acyl derivatives, names with the acid component cited as a separate word ending in 'ate' after the monosaccharide name are preferred to names using *O*-acyl group prefixes. However when the ose ending is changed (e.g. to denote a glycosyl or an acid function having seniority over an ester) *O*-acyl prefixes are required. *O*-Alkyl derivatives are always expressed by prefixes.

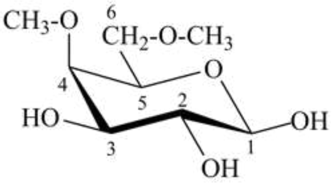
Examples:



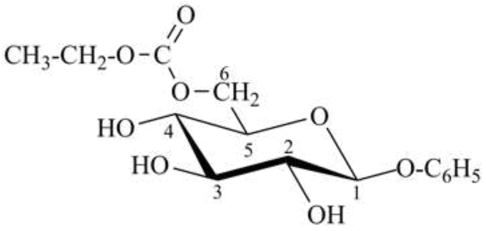
6-*O*-trityl-β-D-glucopyranose 2,4-diacetate



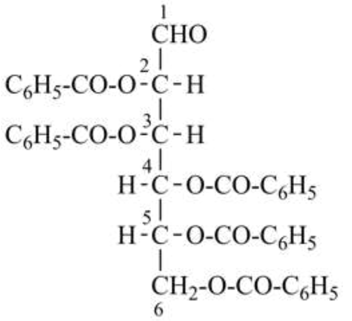
2,3,4,6-tetra-*O*-methyl-β-D-glucopyranose



4,6-di-*O*-methyl-β-D-galactoyranose



phenyl β-D-glucopyranoside 6-(ethyl carbonate)



D-mannose 2,3,4,5,6-pentabenzoate

P-102.5.6.1.2 Phosphoric acid esters

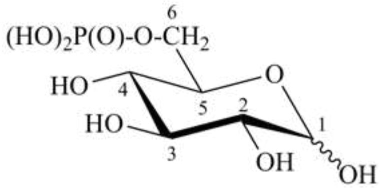
Esters of sugars with phosphoric acid are generally termed ‘phosphates’. In biochemical usage, the term ‘phosphate’ indicates the phosphate residue regardless of the state of ionization or the counter ions present. However, systematically the names must differentiate between a true phosphate, $–O\text{-}PO(O^–)_2$, and an acid phosphate, i.e., $-O\text{-}PO(OH)_2$, called a (dihydrogen phosphate). The prefixes ‘phosphono’, for $–PO(OH)_2$, and ‘phosphonato’, for $PO(O^–)_2$, are also used, to denote *O*-phosphonic acid derivatives.

The term ‘phospho’ is used in place of ‘phosphono’ and ‘phosphonato’ in biochemical contexts.

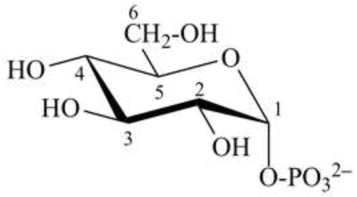
When the sugar is esterified by two or more phosphate groups, the numerical terms ‘bis’, ‘tris’ are used, as ‘bis(phosphate)’, ‘tris(phosphate)’.

Phosphonates are treated in the same way as phosphates.

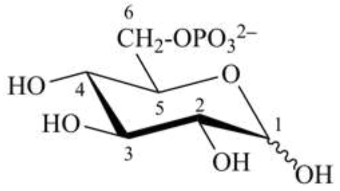
Examples:



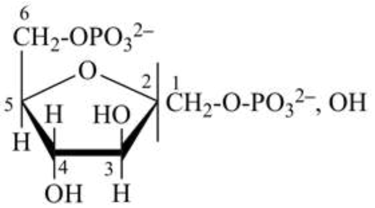
D-glucopyranose 6-(dihydrogen phosphate)
6-*O*-phosphono-D-glucopyranose



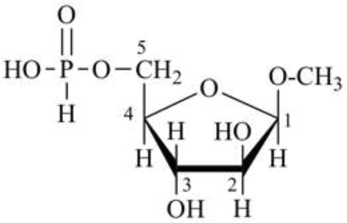
α-D-glucopyranosyl phosphate
α-D-glucopyranose 1-phosphate



D-glucopyranose 6-phosphate
6-*O*-phosphonato-D-glucopyranose



D-fructofuranose 1,6-bis(phosphate)
1,6-di-*O*-phosphonato-D-fructofuranose

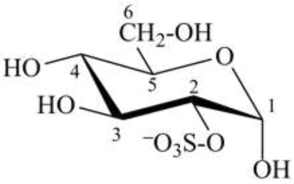


methyl β-D-arabinofuranoside 5-(hydrogen phosphonate)
methyl 5-deoxy-β-D-arabinofuranosid-5-yl hydrogen phosphonate

P-102.5.6.1.3 Esters with sulfuric acid

Esters of sugars with sulfuric acid are named by adding the term ‘sulfate’ after the name of the sugar, with the appropriate locant. The prefixes ‘sulfo’ for $–SO_3H$, and ‘sulfonato’ for $SO_3^–$, can be used to denote *O*-derivatives.

Example:



α-D-glucopyranose 2-sulfate
2-*O*-sulfonato-α-D-glucopyranose

P-102.5.6.2 Glycosides

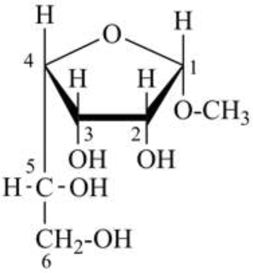
P-102.5.6.2.1 Definitions

Glycose is a less frequently used term for a monosaccharide. Glycosides are mixed acetals (ketals) derived from cyclic forms of monosaccharides, thus, having an *O*-substituted anomeric –OH group, such as –OR. See ref. 27 for a full discussion on the use of the term glycoside.

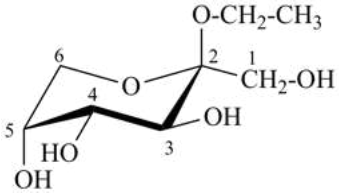
P-102.5.6.2.2 Names

Glycosides are named by using functional class nomenclature. The name of the class ‘glycoside’ is adapted to the name of each cyclic monosaccharide, by changing the letter ‘e’ at the end of the name to ‘ide’, for example glucopyranose becomes glucopyranoside, fructofuranose becomes fructofuranoside. The class name is preceded, as a separate word, by the name of the substituent group that is part of the acetal or ketal function.

Examples:



methyl α-D-gulofuranoside



ethyl β-D-fructopyranoside

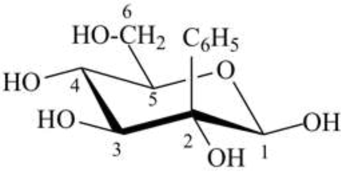
P-102.5.6.3 *C*-Substitution

P-102.5.6.3.1 Substitution at a nonterminal carbon atom
P-102.5.6.3.2 Substitution replacing a nonterminal hydroxy group
P-102.5.6.3.3 Substitution at a terminal carbon atom

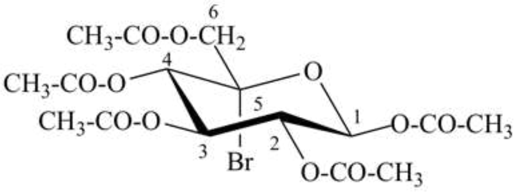
P-102.5.6.3.1 Substitution at a nonterminal carbon atom

The compound is named as a *C*-substituted monosaccharide. The group having priority in accordance with the CIP priority system is regarded as equivalent to –OH for assignment of configuration. Any ambiguity (e.g. at a carbon atom where ring formation occurs) is avoided by using the *R*,*S* system to specify the configuration at the modified chirality center.

Examples:



2-*C*-phenyl-β-D-glucopyranose
(2*R*,3*R*,4*S*,5*S*,6*R*)-6-(hydroxymethyl)-3-phenyloxane-2,3,4,5-tetrol

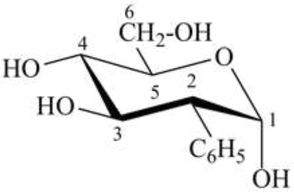


5-*C*-bromo-β-D-glucopyranose pentaacetate
(2*R*,3*R*,4*R*,5*S*,6*S*)-6-[(acetyloxy)methyl]-6-bromooxane-2,3,4,5-tetrayl tetraacetate

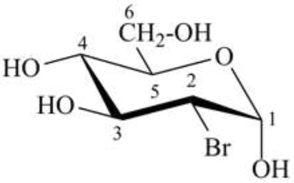
P-102.5.6.3.2 Substitution replacing a nonterminal hydroxy group

The compound is named as a substituted derivative of a deoxy sugar. The group replacing the –OH group determines the configuration. Any potential ambiguity must be dealt with by the use of the *R*,*S* system. The *R*,*S* system must be used to assign the preferred configuration of a chirality center twice substituted; this method is preferable to that establishing the configuration by making the substituent with high CIP priority equivalent to the –OH group.

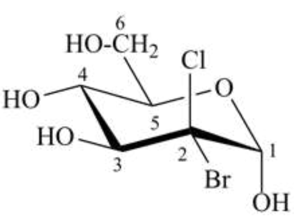
Examples:



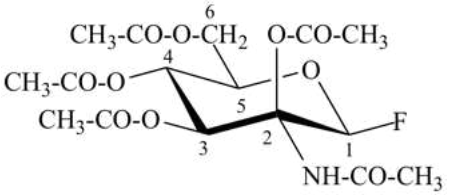
2-deoxy-2-phenyl-α-D-glucopyranose
2-deoxy-2-*C*-phenyl-α-D-glucopyranose
(2*R*)-2-deoxy-2-phenyl-α-D-*arabino*-hexopyranose
(2*S*,3*R*,4*R*,5*S*,6*R*)-6-(hydroxymethyl)-3-phenyloxane-2,4,5-triol



2-bromo-2-deoxy-α-D-glucopyranose



(2*R*)-2-bromo-2-chloro-2-deoxy-α-D-*arabino*-hexopyranose
2-bromo-2-chloro-2-deoxy-α-D-glucopyranose
(2*S*,3*R*,4*S*,5*S*,6*R*)-3-bromo-3-chloro-6-(hydroxymethyl)oxane-2,4,5-triol

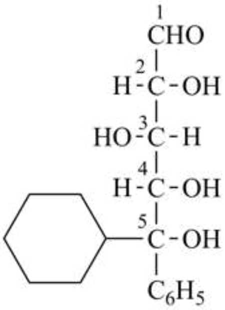


2-*C*-acetamido-2,3,4,6-tetra-*O*-acetyl-β-D-mannopyranosyl fluoride
(2*S*,3*S*,4*S*,5*R*,6*R*)-3-acetamido-6-[(acetyloxy)methyl]-2-fluorooxane-3,4,5-triyl triacetate

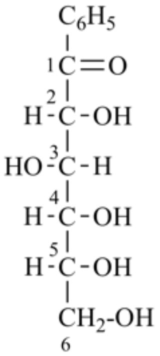
P-102.5.6.3.3 Substitution at a terminal carbon atom

Substitution at a terminal carbon atom of a carbohydrate chain creates a new chirality center; the configuration is indicated by the '*R/S*' system. Preferred names are formed substitutively.

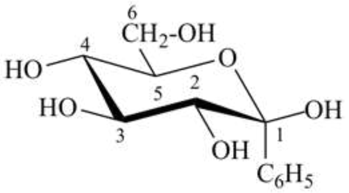
Examples:



(5*R*)-5-*C*-cyclohexyl-5-*C*-phenyl-D-xylose
(2*R*,3*S*,4*S*,5*R*)-5-cyclohexyl-2,3,4,5-tetrahydroxy-5-phenylpentanal



1-phenyl-D-glucose
(2*R*,3*S*,4*R*,5*R*)-2,3,4,5,6-pentahydroxy-1-phenylhexan-1-one



1-*C*-phenyl-β-D-glucopyranose
(2*R*,3*R*,4*S*,5*S*,6*R*)-6-(hydroxymethyl)-2-phenyloxane-2,3,4,5-tetrol

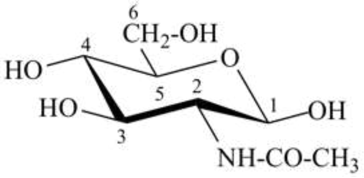
P-102.5.6.4 *N*-Substitution

Substitution at the –NH2 group of an amino sugar is dealt with in two different ways:

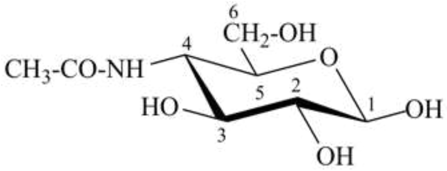
(1) The whole substituted amino group is designated as a prefix as in 2-acetamido-2-deoxy-D-glucose or 2- (butylamino)-2-deoxy-D-glucose.

(2) If the amino sugar has a retained trivial name, the substitution is indicated by a prefix preceded by the capital italicized letter *N*.

Examples:



2-acetamido-2-deoxy-β-D-glucopyranose
N-acetyl-β-D-glucosamine



4-acetamido-4-deoxy-β-D-glucopyranose

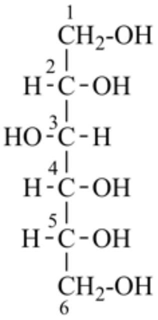
P-102.5.6.5 Alditols

Alditols are named by changing the ending ‘ose’ in the name of the corresponding aldose into ‘itol’.

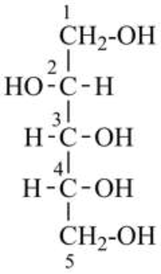
P-102.5.6.5.1 Choice of a parent structure

When the same alditol can be derived from either of two different aldoses, or from an aldose or a ketose, the recommended structure is derived from Rule P-102.4, with the exception of the retained names fucitol and rhamnitol.

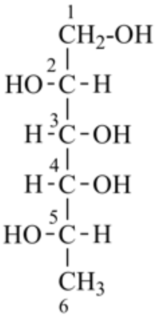
Examples:



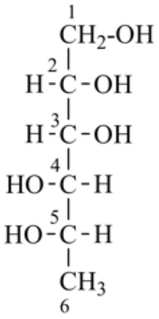
D-glucitol
(not L-gulitol)



D-arabinitol
(not D-lyxitol)



L-fucitol
1-deoxy-D-galactitol

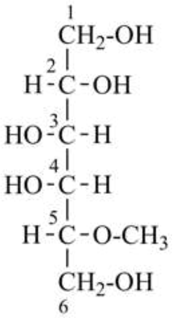


L-rhamnitol
1-deoxy-L-mannitol

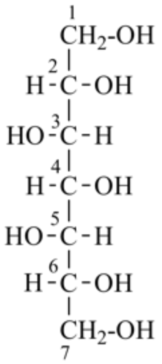
P-102.5.6.5.2 *meso*-Forms

The prefix ‘*meso*’ may be included in the preferred names of erythritol, ribitol and galactitol. The stereodescriptor ‘D’ or ‘L’ must be given when a derivative of a ‘*meso*’ form has become asymmetric by substitution. It is also necessary to use the stereodescriptor ‘D’ or ‘L’ in the case where there are more than four contiguous chirality centers.

Examples:



5-*O*-methyl-D-galactitol
(a ‘D’ configuration is senior to ‘L’; see P-102.4)



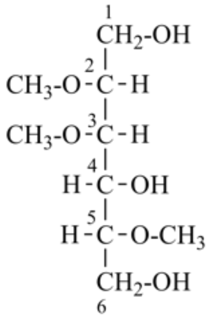
meso-D-*glycero*-L-*ido*-heptitol
(a ‘D’ configuration is senior to ‘L’: see P-102.4)
(2*R*,3*S*,4*r*,5*R*,6*S*)-heptane-1,2,3,4,5,6,7-heptol
(note that locant ‘1’ must be shifted to the other end of the alditol)

P-102.5.6.5.3 Choice of parent structure for substituted alditols

The parent structure must have:

(a) the lowest locants for substituent prefixes in accordance with criterion (e) in Rule P-102.4;

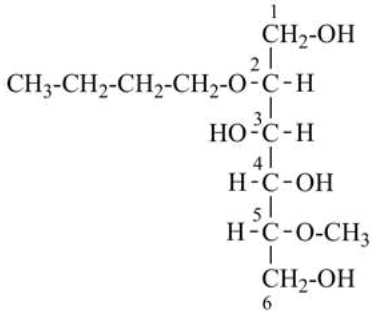
Example:



2,3,5-tri-*O*-methyl-D-mannitol
(not 2,4,5-tri-*O*-methyl-D-mannitol)

(b) the lowest locant for the first cited substituent in alphanumerical order, in accordance with criterion (f) in Rule P-102.4.

Example:

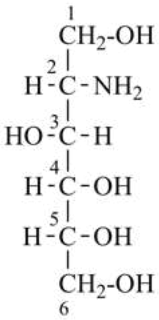


2-*O*-butyl-5-*O*-methyl-D-mannitol
(not 5-*O*-butyl-2-*O*-methyl-D-mannitol)

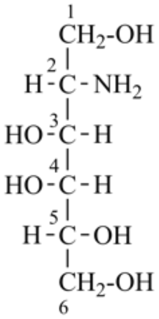
P-102.5.6.5.4 Aminoalditols

Alditols derived from galactosamine and glucosamine are aminoalditols. They have retained names, galactosaminitol and glucosaminitol, respectively.

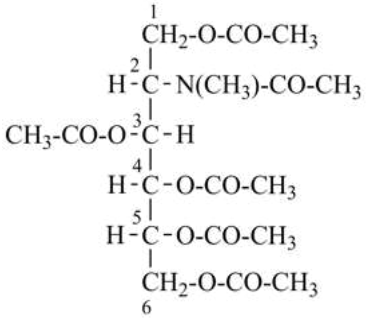
Examples:



D-glucosaminitol
2-amino-2-deoxy-D-glucitol



D-galactosaminitol
2-amino-2-deoxy-D-galactitol



2-deoxy-2-(*N*-methylacetamido)-D-glucitol 1,3,4,5,6-pentaacetate

P-102.5.6.6 Monosaccharide carboxylic acids

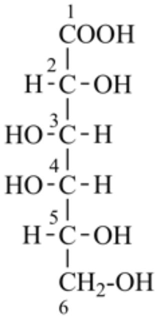
P-102.5.6.6.1 Classifiations

P-102.5.6.6.2 Aldonic acids. Monocarboxylic acids formally derived from aldoses by oxidation of the aldehydic group to a carboxylic acid are called aldonic acids.
P-102.5.6.6.3 Ketoaldonic acids. Oxo carboxylic acids formally derived from aldonic acids by oxidation of a secondary –CHOH group to a carbonyl group are called ketoaldonic acids.
P-102.5.6.6.4 Uronic acids. Carboxylic acids formally derived from aldoses by oxidation of the terminal –CH_2OH group to a carboxy group are called uronic acids.
P-102.5.6.6.5 Aldaric acids. Carboxylic acids formed by the oxidation of both terminal groups (–CHO and –CH_2OH) of aldoses to carboxy groups are called aldaric acids.

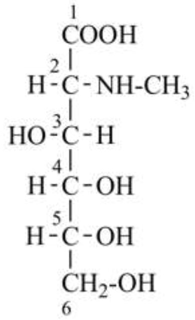
P-102.5.6.6.2 Aldonic acids

Aldonic acids are divided into aldotrionic acids, aldotetronic acids, etc. according to the number of carbon atoms in the chain. The names of individual compounds are formed by changing the ending ‘ose’ of the retained or systematic name of the aldose to ‘onic acid’. The locant 1 is assigned to the carboxy group.

Examples:



D-galactonic acid

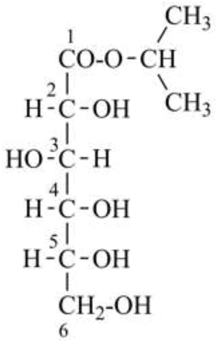


2-deoxy-2-(methylamino)-D-gluconic acid

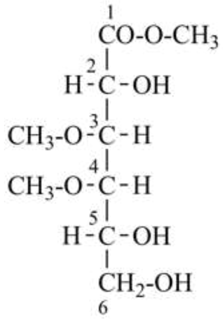
P-102.5.6.6.2.1 Derivatives of aldonic acids

Aldonic acids are treated as carboxylic acids having a retained name. They can form salts, esters, anhydrides, acyl groups and acid halides and pseudohalides, amides, hydrazides, nitriles and chalcogen analogues as described in Sections P-65 and P-66 for systematic nomenclature.

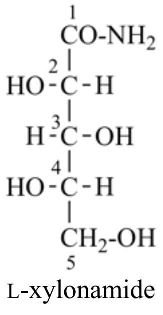
Examples:



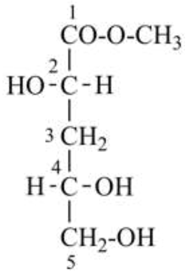
propan-2-yl D-gluconate



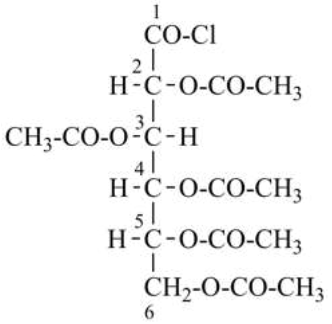
methyl 3,4-di-*O*-methyl-D-galactonate



L-xylonamide



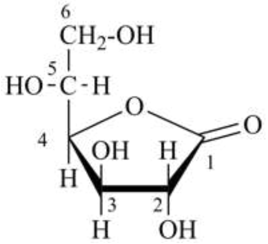
methyl 3-deoxy-D-*threo*-pentonate



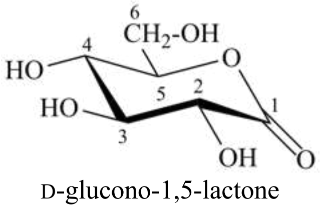
2,3,4,5,6-penta-*O*-acetyl-D-gluconoyl chloride

P-102.5.6.6.2.2 Lactones and lactams are named by adapting Rules P-65.6.3.5.1 and P-66.1.5, respectively. Two locants are used before the lactone or lactam term: the first one is the locant 1 denoting the carboxy group position; the second locant denotes the position of attachment on the carbon chain. To name lactams, the amino group, –NH_2, must be generated and cited. The use of Greek letters to indicate the size of a lactone or lactam ring is not recommended. Names can also be formed substitutively on the basis of heterocyclic rings in accordance with the rules described in Chapters P-1 through P-9.

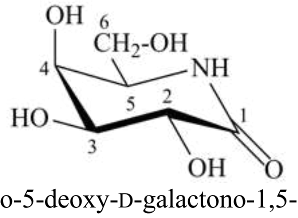
Examples:



D-glucono-1,4-lactone
(3*R*,4*R*,5*R*)-5-[(1*R*)-1,2-dihydroxyethyl]-3,4-dihydroxyoxolan-2-one



D-glucono-1,5-lactone
(3*R*,4*S*,5*S*,6*R*)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-one

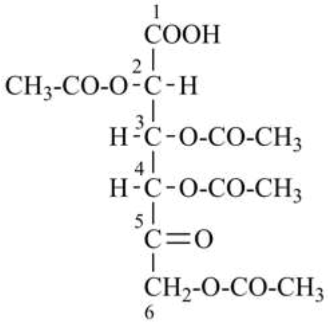


5-amino-5-deoxy-D-galactono-1,5-lactam
(3*R*,4*S*,5*S*,6*R*)-3,4,5-trihydroxy-6-(hydroxymethyl)piperidin-2-one

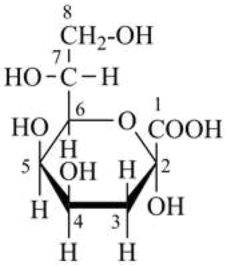
P-102.5.6.6.3 Ketoaldonic acids

P-102.5.6.6.3.1 Names of individual ketoaldonic acids are formed by changing the ending ‘ulose’ in the name of the corresponding ketose to ‘ulosonic acid’, preceded by the locant of the ketonic group. The numbering starts at the carboxy group.

Examples:



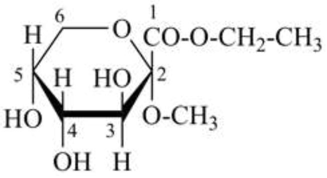
2,3,4,6-tetra-*O*-acetyl-D-*arabino*-hex-5-ulosonic acid
(2*S*,3*R*,4*S*)-2,3,4,6-tetrakis(acetyloxy)-5-oxohexanoic acid



3-deoxy-α-D-*manno*-oct-2-ulopyranosonic acid
(2*R*,4*R*,5*R*,6*R*)-6-[(1*R*)-1,2-dihydroxyethyl]-2,4,5-trihydroxyoxane-2-carboxylic acid

P-102.5.6.6.3.2 Glycosides of ketoaldonic acids are named by changing the component 'pyranose' into 'pyranoside' in the name, to give '-ulopyranosidonic acid'. Names of derivatives of ketoaldonic acids are formed as described in P-102.5.6.6.2 for aldonic acids. When a glycoside is esterified, parentheses are used to isolate the glycosidic portion of the name.

Example:

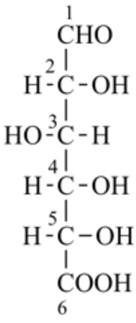


ethyl (methyl α-D-fructopyranosid)onate
ethyl (methyl α-D-*arabino*-hex-2-ulopyranosid)onate
ethyl (2*R*,3*S*,4*R*,5*R*)-3,4,5-trihydroxy-2-methoxyoxane-2-carboxylate

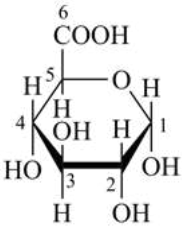
P-102.5.6.6.4 Uronic acids

P-102.5.6.6.4.1 Names of individual uronic acids are formed by changing the ending 'ose' in the retained or systematic name of the corresponding aldose to 'uronic acid'. The numbering of the aldose is kept intact; the locant '1' is still assigned to the (potential) aldehydic group.

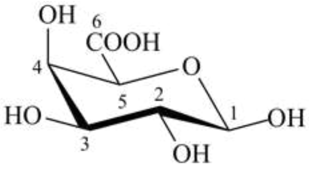
Examples:



D-glucuronic acid



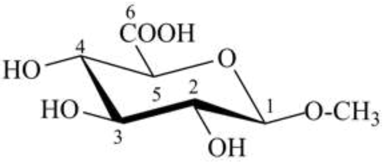
α-D-glucopyranuronic acid



β-D-galactopyranuronic acid

P-102.5.6.6.4.2 Glycosides of uronic acids are named by changing the ‘pyran’ component in the name of the acid to ‘pyranoside’, with elision of the final letter ‘e’, to give ‘pyranosiduronic acid’.

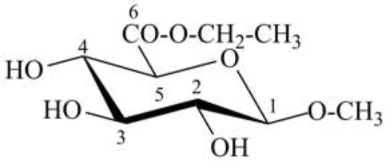
Example:



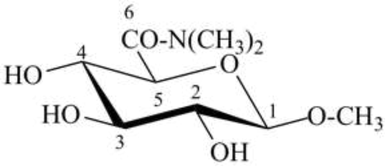
methyl β-D-glucopyranosiduronic acid

P-102.5.6.6.4.3 Derivatives of uronic acid are named as indicated in P-102 and P-65 and P-66.

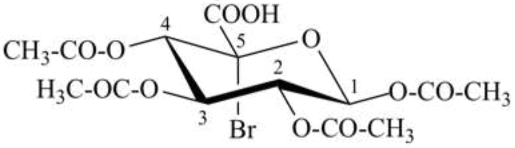
Examples:



ethyl (methyl β-D-glucopyranosid)uronate



N,*N*-dimethyl(methyl β-D-glucopyranosid)uronamide

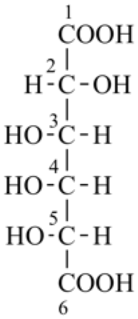


(5*R*)-1,2,3,4-tetra-*O*-acetyl-5-*C*-bromo-α-D-*xylo*-hexopyranuronic acid
(2*R*,3*S*,4*R*,5*R*,6*R*)-3,4,5,6-tetrakis(acetyloxy)-2-bromooxane-2-carboxylic acid

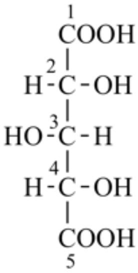
P-102.5.6.6.5 Aldaric acids

P-102.5.6.6.5.1 Names of aldaric acids are formed by changing the ‘ose’ ending in retained or systematic names of parent aldoses to ‘aric acid’. Choice of a parent structure is made in accordance with P-102.4 and P-102.5.6.5.1. The stereodescriptor ‘*meso*’ may be added for sake of clarity to the names of the appropriate aldaric acids.

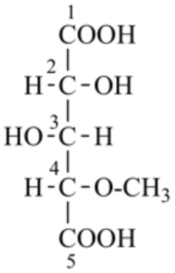
Examples:



L-altraric acid
(not L-talaric acid)



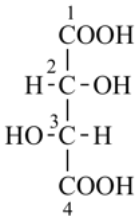
meso-xylaric acid



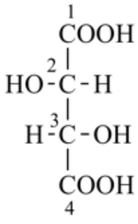
4-*O*-methyl-D-xylaric acid
(not 2-*O*-methyl-L-xylaric acid)

P-102.5.6.6.5.2 Tartaric acid is the retained name to describe the aldaric acids corresponding to the parent aldoses, erythrose and threose. '*R*' and '*S*' are preferred stereodescriptors for denoting the configuration of tartaric acid. Salts and esters are referred to as tartrates.

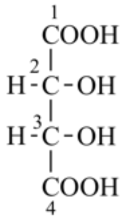
Examples:



(2*R*,3*R*)-2,3-dihydroxybutanedioic acid
(2*R*,3*R*)-tartaric acid
L-threaric acid
(+)-tartaric acid



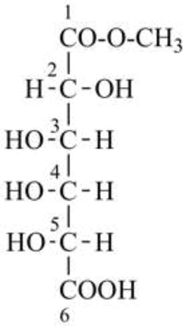
(2*S*,3*S*)-2,3-dihydroxybutanedioic acid
(2*S*,3*S*)-tartaric acid
D-threaric acid
(–)-tartaric acid


1
COOH
2
H-C-OH
3
H-C-OH
COOH
4

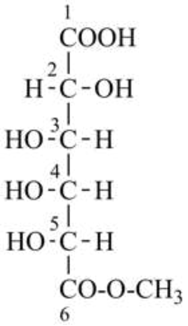
(2*R*,3*S*)-2,3-dihydroxybutanedioic acid
(2*R*,3*S*)-tartaric acid
erythraric acid
meso-tartaric acid

P-102.5.6.6.5.3 Derivatives of aldaric acids formed by modifying the carboxy group (into esters, amides, hydrazides, nitriles, amic acids, etc.) are named by the methods described in P-102.5.6.6.2.1, P-65 and P-66.

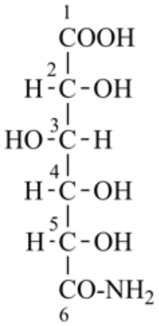
Examples:


1
CO-O-CH3
2
H-C-OH
3
HO-C-H
4
HO-C-H
5
HO-C-H
COOH
6

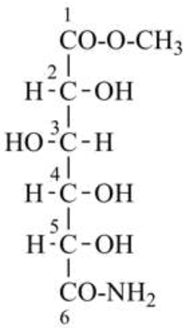
1-methyl hydrogen L-altrarate


1
COOH
2
H-C-OH
3
HO-C-H
4
HO-C-H
5
HO-C-H
CO-O-CH3
6

6-methyl hydrogen L-altrarate


1
COOH
2
H-C-OH
3
HO-C-H
4
H-C-OH
5
H-C-OH
CO-NH2
6

6-amino-6-deoxy-6-oxo-D-gluconic acid
D-glucar-6-amic acid


1
CO-O-CH3
2
H-C-OH
3
HO-C-H
4
H-C-OH
5
H-C-OH
CO-NH2
6

methyl 6-amino-6-deoxy-6-oxo-D-gluconate
1-methyl D-glucar-6-amate

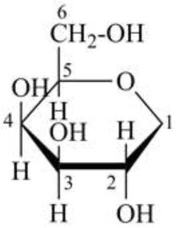
P-102.5.6.7 Anhydrides

Anhydrides are intramolecular or intermolecular derivatives of monosaccharides.

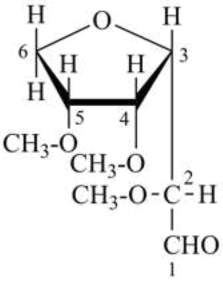
P-102.5.6.7.1 Intramolecular anhydrides

An intramolecular ether (commonly called an intramolecular anhydride), formally arising by elimination of water from two hydroxy groups of a single molecule of a monosaccharide (aldose, ketose) or monosaccharide derivative, is named by adding the detachable prefix ‘anhydro’, preceded by a pair of locants identifying the two hydroxy groups, to the name of the monosaccharide.

Examples:



1,5-anhydro-D-galactitol
(2*R*,3*R*,4*R*,5*S*)-2-(hydroxymethyl)oxane-3,4,5-triol

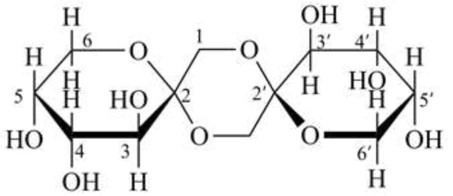


3,6-anhydro-2,4,5-tri-*O*-methyl-D-glucose
(2*R*)-2-[(2*S*,3*R*,4*R*)-3,4-dimethoxyoxolan-2-yl]-2-methoxyacetaldehyde

P-102.5.6.7.2 Intermolecular anhydrides

The cyclic product of condensation of two monosaccharide molecules with elimination of two molecules of water (commonly called an intermolecular anhydride) is named by placing the term ‘dianhydride’ after the names of the two parent monosaccharides. When the two parents are different, the senior parent, according to the selection criteria for selecting the parent structure (see P-102.4), is cited first. The position of each anhydride link is indicated by a pair of locants showing the position of the two hydroxy groups involved, the locants relating to one monosaccharide (in a mixed anhydride, the second monosaccharide named) are primed. The pair of locants immediately precedes the term ‘dianhydride’.

Example:



α-D-fructopyranose β-D-fructopyranose 1,2′:1′,2-dianhydride
[α-D-fructopyranose is cited first; according to P-102.4 (c), α precedes β]
(3*R*,4*R*,5*S*,6*R*,9*S*,12*R*,13*R*,14*S*)-1,7,10,15-tetraoxadispiro[$5.2.5^{9}.2^{6}$]hexadecane-3,4,5,12,13,14-hexol

P-102.6 MONOSACCHARIDES AND DERIVATIVES AS SUBSTITUENT GROUPS

P-102.6.1 Glycosyl groups
P-102.6.2 Substituent groups other than glycosyl groups

P-102.6.1 Glycosyl groups

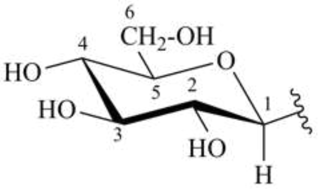
P-102.6.1.1 Glycosyl groups
P-102.6.1.2 *O*-Glycosyl compounds
P-102.6.1.3 *N*-Glycosyl compounds (glycosylamines)
P-102-6.1.4 *C*-Glycosyl compounds
P-102.6.1.5 Glycosyl halides, pseudohalides and esters

P-102.6.1.1 Glycosyl groups

P-102.6.1.1.1 Substituent groups formed by removal of the anomeric hydroxy group from a cyclic monosaccharide are named by replacing the final letter 'e' of the monosaccharide name by 'yl'. The term 'glycosyl residue' is used in the nomenclature of carbohydrates. Terms of this nature are widely used in naming glycosides, when they are not the parent structures, and oligosaccharides.

No locant is added to the name of the substituent to indicate the position of the free valence. A sinuous line denotes the free valence, as recommended for cyclic substituent groups in systematic nomenclature.

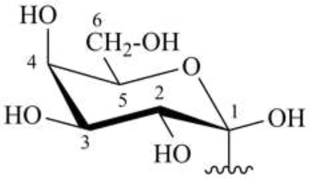
Examples:



β-D-glucopyranosyl
(the hydrogen atom at position 1 is shown)

P-102.6.1.1.2 When the free valence is formed at carbon '1' by subtraction of a hydrogen atom, the substituent group is named as a glycosyl group but the presence of the hydroxy group is denoted by substitution at carbon '1'. In this case, the stereodescriptor 'α' or 'β' refers to the free valence, not to the –OH group.

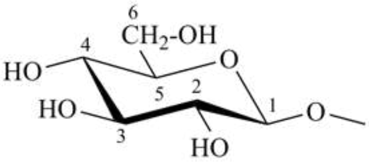
Example:



1-hydroxy-α-D-galactopyranosyl

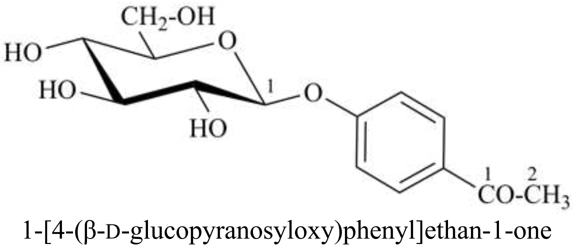
P-102.6.1.2 *O*-Glycosyl compounds

The substituent group formed by removal of a hydrogen atom from the anomeric –OH group is considered as a compound substituent group formed by the 'glycosyl' group and an 'oxy' group. In the examples, names are formed by using the seniority of class to determine the principal characteristic group to be assigned to the monosaccharide or to the aglycone component.

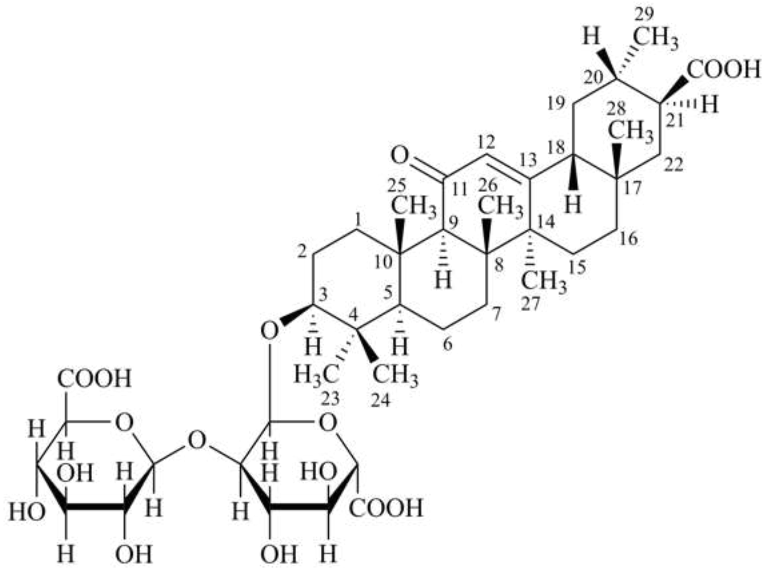


β-D-glucopyranosyloxy

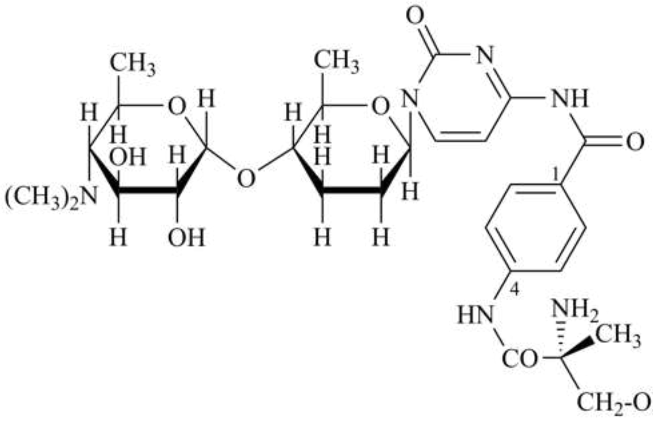
Examples:



1-[4-(β-D-glucopyranosyloxy)phenyl]ethan-1-one
[not 4′-(β-D-glucopyranosyloxy)acetophenone;
acetophenone cannot be substituted (see P-64.2.1.2)]
(not 4-acetylphenyl β-D-glucopyranoside;
a ketone is senior to a hydroxy compound)



21β-carboxy-11-oxo-30-norolean-12-en-3β-yl (2-*O*-β-D-glucopyranosyluronic acid)-α-D-glucopyranosiduronic acid



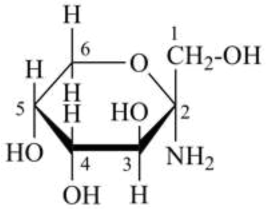
4-[(2*R*)-2-amino-3-hydroxy-2-methylpropanamido]-*N*-{1-[(2*R*,5*S*,6*R*)-5-{[4,6-dideoxy-4-(dimethylamino)-α-D-glucopyranosyl]oxy}-6-methyloxan-2-yl]-2-oxo-1,2-dihydropyrimidin-4-yl}benzamide

Explanation: the principal function is an amide; the cyclic amide, benzamide, is senior to the acyclic amide, propanamide.

P-102.6.1.3 *N*-Glycosyl compounds (glycosylamines)

N-Glycosyl derivatives are named as glycosylamines.

Example:

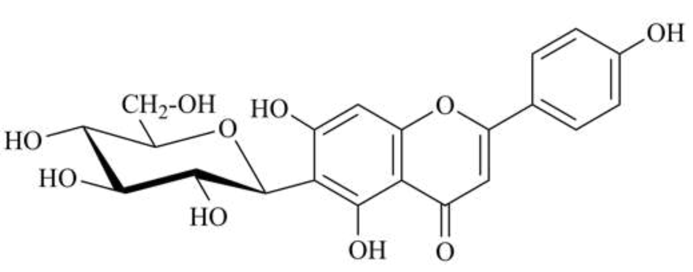


α-D-fructopyranosylamine

P-102.6.1.4 *C*-Glycosyl compounds

Compounds arising formally from the elimination of water from the glycosidic hydroxy group and a hydrogen atom bound to a carbon atom (thus creating a C-C bond) are named using the appropriate glycosyl group.

Example:

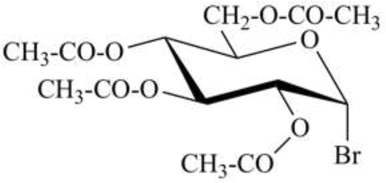


6-(β-D-glucopyranosyl)-5,7-dihydroxy-2-(4-hydroxyphenyl)-4*H*-chromen-4-one
6-(β-D-glucopyranosyl)-5,7-dihydroxy-2-(4-hydroxyphenyl)-4*H*-1-benzopyran-4-one
6-(β-D-glucopyranosyl)-4′,5,7-dihydroxyflavone

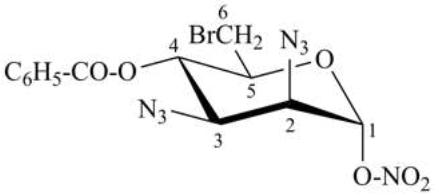
P-102.6.1.5 Glycosyl halides, pseudohalides and esters

Glycosyl halides and pseudohalides are named by using functional class nomenclature, by adding, as a separate word, the class name 'chloride', 'isocyanate', etc. to the name of the appropriate glycosyl group. Esters of oxoacids in position 1 are treated as described for esters at other positions (see P-102.5.6.1).

Examples:


CH2-O-CO-CH3
O
CH3-CO-O
CH3-CO-O
O
CH3-CO
Br

2,3,4,6-tetra-*O*-acetyl-α-D-glucopyranosyl bromide

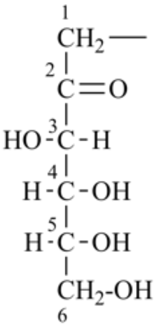

6
4 BrCH2 N3
O
C6H5-CO-O
5
N3
2
1
3
O-NO2

2,3-diazido-6-bromo-2,3,6-trideoxy-α-D-mannopyranose 4-benzoate 1-nitrate

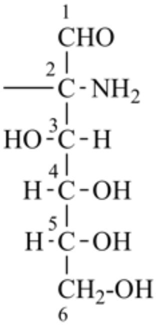
P-102.6.2 Substituent groups other than glycosyl groups

A hydrogen atom may be removed from any position of a monosaccharide other than C-1. This formation of a free valence is denoted by the suffix 'yl', but a locant is necessary to indicate the position of the free valence and to distinguish such a name from that of glycosyl substituents for which the locant '1' is omitted. These prefixes can be formed by replacing the final letter 'e' of the systematic or trivial name of a monosaccharide by *n*-*C*-yl, *n*-*O*-yl. The symbol '*C*' is omitted when the free valence is derived from a position at which hydrogen atoms only are attached.

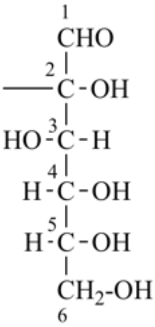
Examples:


1
CH2
2
C=O
3
HO-C-H
4
H-C-OH
5
H-C-OH
CH2-OH
6

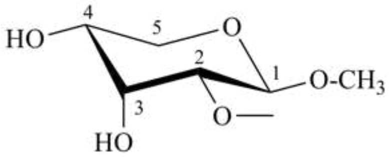
1-deoxy-D-fructos-1-yl


1
CHO
2
C-NH2
3
HO-C-H
4
H-C-OH
5
H-C-OH
CH2-OH
6

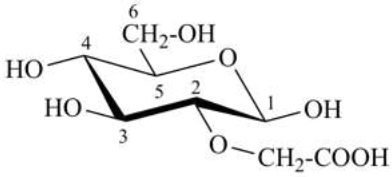
2-amino-2-deoxy-D-glucos-2-*C*-yl


1
CHO
2
C-OH
3
HO-C-H
4
H-C-OH
5
H-C-OH
CH2-OH
6

D-glucos-2-*C*-yl



methyl β-D-ribopyranosid-2-*O*-yl



(β-D-glucopyranos-2-*O*-yl)acetic acid
(not 2-*O*-(carboxymethyl)-β-D-glucopyranose;
this name is not constructed according to P-102.6.1.2;
a carboxylic acid is senior to a hydroxy compound)

P-102.7 DISACCHARIDES AND OLIGOSACCHARIDES

Names of disaccharides and oligosaccharides are formed by the principles, rules, and conventions described above for monosaccharides.

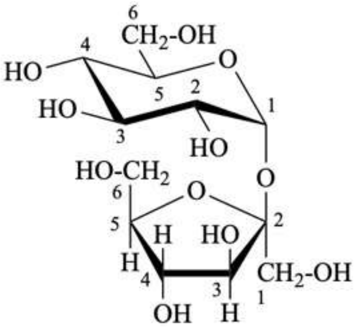
P-102.7.1 Disac10charides
P-102.7.2 Oligosaccharides

P-102.7.1 Disaccharides

P-102.7.1.1 Disaccharides without a free hemiacetal group

Disaccharides which can be regarded as formed by elimination of one molecule of water from two glycosidic (anomeric) hydroxy groups, are named as glycosyl glycosides. The parent (cited as the 'glycoside') is chosen in accordance with criteria described in P-102.4. Both anomeric descriptors must be cited in the name.

Example:



β-D-fructofuranosyl α-D-glucopyranoside
(not α-D-glucopyranosyl β-D-fructofuranoside
fructo precedes gluco in the alphabetical order)
sucrose (trivial name)

P-102.7.1.2 Disaccharides with a free hemiacetal group

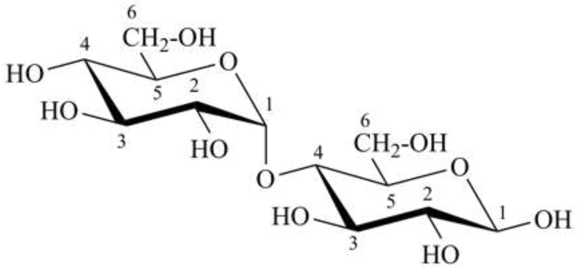
Disaccharides which can be regarded as formed by elimination of one molecule of water from one glycosidic (anomeric) hydroxy group and one alcoholic hydroxy group, are named as glycosylglycoses. Locants and anomeric descriptors must be cited in the full name.

There are two established methods for citing locants:

(1) in parentheses between the components with an arrow going from the locant of the glycosyl component to that of the glycose component;

(2) at the front of the glycosyl component.

Example:



(1) α-D-glucopyranosyl-(1→4)-β-D-glucopyranose
(2) 4-*O*-α-D-glucopyranosyl-β-D-glucopyranose
β-maltose (trivial name;
not β-D-maltose)

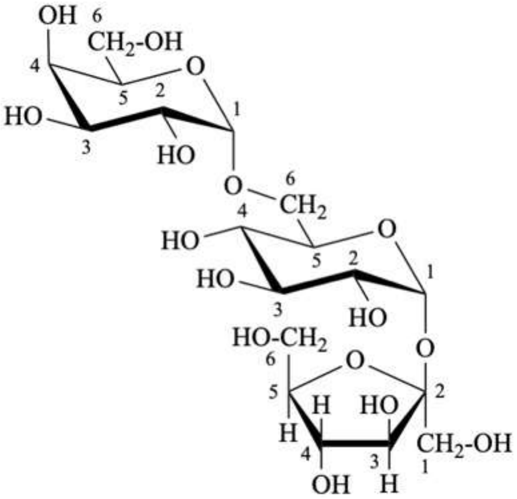
P-102.7.2 Oligosaccharides

Oligosaccharides are multicomponent saccharides generally with more than two monosaccharide units According to the number of units, they are called trisaccharides, tetrasaccharides, etc. The number of units involved before they become polysaccharides is not defined.

P-102.7.2.1 Oligosaccharides without a free hemiacetal group

A trisaccharide, for example, is named as a glycosylglycosyl glycoside or glycosyl glycosylglycoside as required. A choice between the two residues linked through their anomeric positions for citation as the 'glycoside' portion can be made on the basis of P-102.4. Alternatively, a sequential (end-to-end) naming approach may be used, regardless of P-102.4. The name is formed by the preferred method for naming disaccharides.

Example:

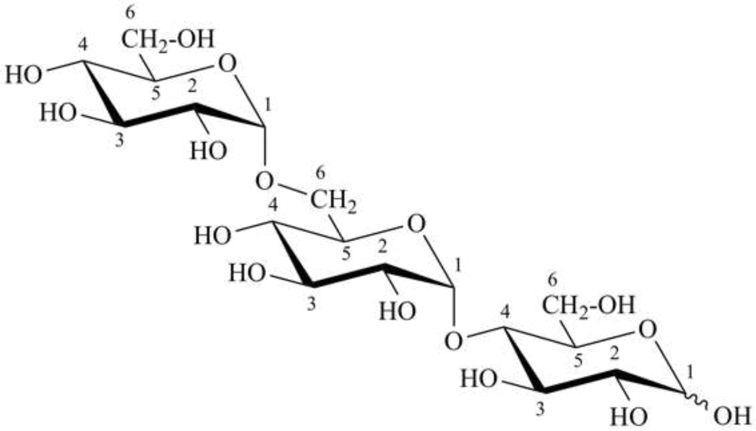


β-D-fructofuranosyl α-D-galactopyranosyl-(1→6)-α-D-glucopyranoside
(glucose, not fructose, is selected as the 'glycoside')
α-D-galactopyranosyl-(1→6)-α-D-glucopyranosyl β-D-fructofuranoside (sequential method)
raffinose (trivial name)

P-102.7.2.2 Oligosaccharides with a free hemiacetal group

An oligosaccharide of this type is named as a glycosyl[glycosyl]$_n$glycose, the 'glycose' portion being the parent. The conventional depiction has the 'glycose' portion on the right. Names are formed as described in P-102.7.2.1.

Example:



α-D-glucopyranosyl-(1→6)-α-D-glucopyranosyl-(1→4)-D-glucopyranose
panose (trivial name)

P-103 AMINO ACIDS AND PEPTIDES

P-103.0 Introduction
P-103.1 Names, numbering, and configuration specification of amino acids
P-103.2 Derivatives of amino acids
P-103.3 Nomenclature of peptides

P-103.0 INTRODUCTION

This Section describes the nomenclature of amino acids that constitute the building blocks of peptides and proteins. They are functional parents having retained names listed in Table 10.4. Less common amino acids also have retained names (see Table 10.5). The nomenclature of amino acids is composed of two types of names: names based on retained names for functional parents, with a limited capacity of functionalization and substitution, and systematic substitutive names for all other compounds.

The nomenclature of these amino acids and peptides is described in the document entitled ‘Nomenclature and Symbolism for Amino Acids and Peptides’ (ref. 18). A document covering the nomenclature of cyclic peptides is in preparation. In this Section, the nomenclature of these amino acids and peptides is restricted to their derivatives outside the field of peptides and proteins.

P-103.1 NAMES, NUMBERING, AND CONFIGURATION SPECIFICATION OF AMINO ACIDS

P-103.1.1 Retained and systematic names
P-103.1.2 Numbering of α-amino carboxylic acids
P-103.1.3 Configuration of α-amino carboxylic acids

P-103.1.1 Retained and systematic names

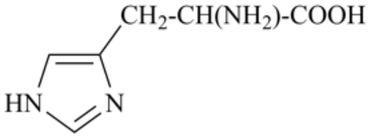
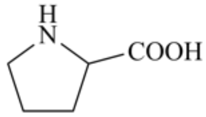
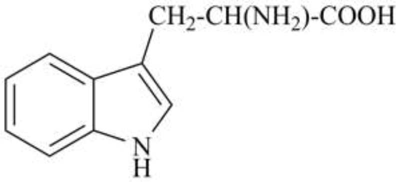
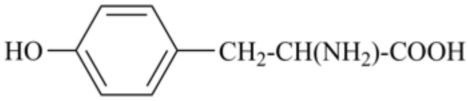
P-103.1.1.1 Retained names of the ‘common’ amino acids
P-103.1.1.2 Retained names of ‘less common’ amino acids
P-103.1.1.3 Systematic substitutive names

P-103.1.1.1 Retained names of the ‘common’ amino acids

The retained names of the α-amino acids that are commonly found in proteins and are represented in the genetic code, together with their systematic names, symbols (3-letter and/or 1-letter), and formulas, are given in Table 10.4. Some less common amino acids are discussed in P-103.1.1.2 and listed in Table 10.5.

Table 10.4 Retained names of ‘common’ α-amino acids

Retained name **Systematic name**	**Symbols** **3-letter**	 **1-letter**	**Formula**
alanine 2-aminopropanoic acid	Ala	A	CH_3-CH(NH_2)-COOH
arginine 2-amino-5-(carbamimidoylamino)pentanoic acid	Arg	R	H_2N-C(=NH)-NH-[CH_2]$_3$-CH(NH_2)-COOH
asparagine	Asn	N	H_2N-CO-CH_2-CH(NH_2)-COOH

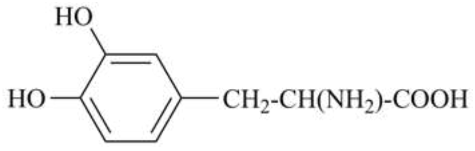
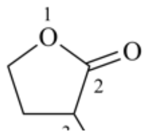
2,4-diamino-4-oxobutanoic acid			
aspartic acid aminobutanedioic acid	Asp	D	$HOOC-CH_2-CH(NH_2)-COOH$
cysteine 2-amino-3-sulfanylpropanoic acid	Cys	C	$HS-CH_2-CH(NH_2)-COOH$
glutamine 2,5-diamino-5-oxopentanoic acid	Gln	Q	$H_2N-CO-[CH_2]_2-CH(NH_2)-COOH$
glutamic acid 2-aminopentanedioic acid	Glu	E	$HOOC-[CH_2]_2-CH(NH_2)-COOH$
glycine aminoacetic acid	Gly	G	H_2N-CH_2-COOH
histidine 2-amino-3-(1*H*-imidazol-4-yl)propanoic acid	His	H	
isoleucine *rel*-(2*R*,3*R*)-2-amino-3-methylpentanoic acid (see P-103.1.3.2.1 for configuration specification)	Ile	I	$CH_3-CH_2-CH(CH_3)-CH(NH_2)-COOH$
leucine 2-amino-4-methylpentanoic acid	Leu	L	$(CH_3)_2CH-CH_2-CH(NH_2)-COOH$
lysine 2,6-diaminohexanoic acid	Lys	K	$H_2N-[CH_2]_4-CH(NH_2)-COOH$
methionine 2-amino-4-(methylsulfanyl)butanoic acid	Met	M	$CH_3-S-[CH_2]_2-CH(NH_2)-COOH$
phenylalanine 2-amino-3-phenylpropanoic acid	Phe	F	$C_6H_5-CH_2-CH(NH_2)-COOH$
proline pyrrolidine-2-carboxylic acid	Pro	P	
serine 2-amino-3-hydroxypropanoic acid	Ser	S	$HO-CH_2-CH(NH_2)-COOH$
threonine *rel*-(2*R*,3*S*)-2-amino-3-hydroxybutanoic acid (see P-103.1.3.2.1 for configuration specification)	Thr	T	$CH_3-CH(OH)-CH(NH_2)-COOH$
tryptophan 2-amino-3-(1*H*-indol-3-yl)propanoic acid	Trp	W	
tyrosine 2-amino-3-(4-hydroxyphenyl)propanoic acid	Tyr	Y	

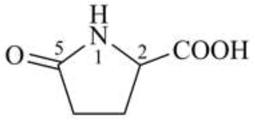
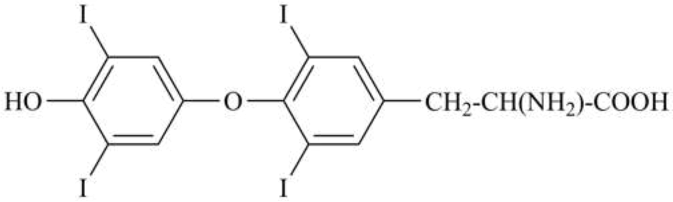
valine 2-amino-3-methylbutanoic acid	Val	V	$(CH_3)_2CH\text{-}CH(NH_2)\text{-}COOH$
unspecified amino acid	Xaa	X	

P-103.1.1.2 Retained names of ‘less common’ amino acids

Several other less common trivial names and their symbols are described in Table 10.5. The publication ‘Nomenclature and symbolism for amino acids and peptides’ (ref. 18) must be consulted for the complete description of the naming of ‘less common’ amino acids.

Table 10.5 Amino acids with trivial names (other than those listed in Table 10.4)

Retained name **Systematic name**	**Symbol**	**Formula**
β-alanine 3-aminopropanoic acid	βAla	$H_2N\text{-}CH_2\text{-}CH_2\text{-}COOH$
alloisoleucine *rel*-(2*R*,3*S*)-2-amino-3-methylpentanoic acid (see P-103.1.3.2.1 for configuration specification)	aIle	$CH_3\text{-}CH_2\text{-}CH(CH_3)\text{-}CH(NH_2)\text{-}COOH$
allothreonine *rel*-(2*R*,3*R*)-2-amino-3-hydroxybutanoic acid (see P-103.1.3.2.1 for configuration specification)	aThr	$CH_3\text{-}CH(OH)\text{-}CH(NH_2)\text{-}COOH$
allysine 2-amino-6-oxohexanoic acid	—	$HCO\text{-}[CH_2]_3\text{-}CH(NH_2)\text{-}COOH$
citrulline N^5-carbamoylornithine	Cit	$NH_2\text{-}CO\text{-}NH\text{-}[CH_2]_3\text{-}CH(NH_2)\text{-}COOH$
cystathionine *S*-(2-amino-2-carboxyethyl)homocysteine	Ala | Hcy	$HOOC\text{-}CH(NH_2)\text{-}CH_2\text{-}CH_2\text{-}S\text{-}CH_2\text{-}CH(NH_2)\text{-}COOH$
cysteic acid 3-sulfoalanine 2-amino-3-sulfopropanoic acid	Cya	$HO_3S\text{-}CH_2\text{-}CH(NH_2)\text{-}COOH$
cystine 3,3′-disulfanediyldialanine	Cys | Cys	$S\text{-}CH_2\text{-}CH(NH_2)\text{-}COOH$ | $S\text{-}CH_2\text{-}CH(NH_2)\text{-}COOH$
dopa 3-hydroxytyrosine	—	
homocysteine 2-amino-4-sulfanylbutanoic acid	Hcy	$HS\text{-}CH_2\text{-}CH_2\text{-}CH(NH_2)\text{-}COOH$
homoserine 2-amino-4-hydroxybutanoic acid	Hse	$HO\text{-}CH_2\text{-}CH_2\text{-}CH(NH_2)\text{-}COOH$
homoserine lactone 3-aminooxolan-2-one	Hsl	

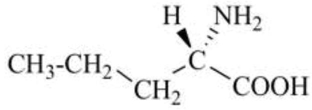
lanthionine 3,3′-sulfanediyldialanine	Ala | Cys	$CH_2\text{-}CH(NH_2)\text{-}COOH$ | $S\text{-}CH_2\text{-}CH(NH_2)\text{-}COOH$
ornithine 2,5-diaminopentanoic acid	Orn	$H_2N\text{-}[CH_2]_3\text{-}CH(NH_2)\text{-}COOH$
5-oxoproline 5-oxopyrrolidine-2-carboxylic acid	Glp	
sarcosine *N*-methylglycine	Sar	$CH_3\text{-}NH\text{-}CH_2\text{-}COOH$
thyroxine *O*-(4-hydroxy-3,5-diiodophenyl)-3,5-diiodotyrosine	Thx	

P-103.1.1.3 Systematic substitutive names

When not denoted by a retained name, amino acids receive systematic substitutive names constructed by applying the principles, rules and conventions of substitutive nomenclature.

Systematic substitutive names are given to homologues of glycine and alanine, for example 2-aminobutanoic acid, 2-aminopentanoic acid (formerly ‘norvaline’) and 2-aminohexanoic acid (formerly ‘norleucine’). The corresponding three-letter symbols are Abu, Ape, and Ahx. The stereodescriptors D and L are used to denote the configuration on C-2. These acids and their symbols are illustrated in 3AA-15.2.3 in ref. 18. The names ‘norvaline’ and ‘norleucine’ are not recommended (see 3AA-15.2.3, ref. 18).

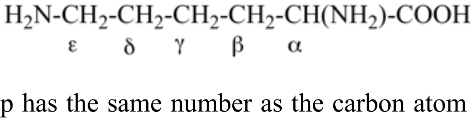
Example:



(2*S*)-2-aminopentanoic acid
(3-letter symbol: Ape)

P-103.1.2 Numbering of α-amino carboxylic acids

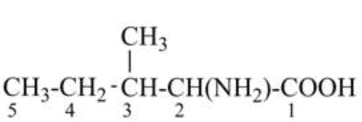
In acyclic amino acids, the carbon atom of the carboxy group next to the carbon atom carrying the amino group is numbered ‘1’. Alternatively, Greek letters may be used, with C-2 designated α.



$$\overset{6}{H_2N\text{-}CH_2}\text{-}\overset{5}{CH_2}\text{-}\overset{4}{CH_2}\text{-}\overset{3}{CH_2}\text{-}\overset{2}{CH}(NH_2)\text{-}\overset{1}{COOH}$$
$$\varepsilon \quad \delta \quad \gamma \quad \beta \quad \alpha$$

A heteroatom in a characteristic group has the same number as the carbon atom to which it is attached, e.g. *N*-2 is on C-2. When such numerals are used as locants they are written as superscripts, e.g. ‘N^2’-acetyllysine (see P-103.2.1).

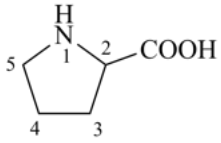
The carbon atoms of the methyl groups of valine are numbered ‘4’ and ‘4′’; likewise, those of leucine are ‘5’ and ‘5′’. Isoleucine is numbered as follows:



$$\underset{5}{CH_3}\text{-}\underset{4}{CH_2}\text{-}\underset{3}{\overset{\overset{\textstyle CH_3}{|}}{CH}}\text{-}\underset{2}{CH}(NH_2)\text{-}\underset{1}{COOH}$$

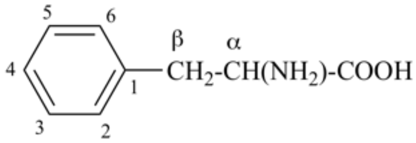
isoleucine

The atoms in proline are numbered as in pyrrolidine, the nitrogen atom being numbered '1', and the carbon atom bonded to the carboxy group is numbered '2'.

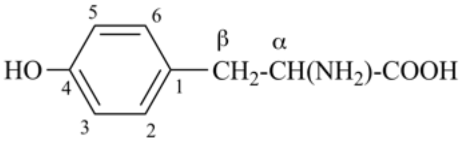

H
N
1
2
5
4
3
COOH

proline

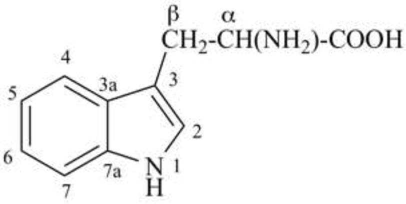
The carbon atoms in the aromatic rings of phenylalanine, tyrosine and tryptophan are numbered as in systematic nomenclature. The carbon atoms of the chains are designated 'α' and 'β' as shown below:


5
6
4
1
3
2
β
α
CH2-CH(NH2)-COOH

phenylalanine

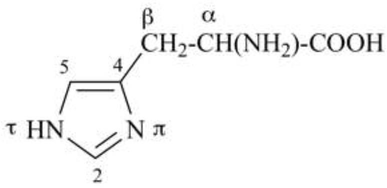

HO
5
6
4
1
3
2
β
α
CH2-CH(NH2)-COOH

tyrosine


β
α
CH2-CH(NH2)-COOH
4
3a
3
5
2
6
7a
N 1
H
7

tryptophan

A special fixed numbering, composed of numerals and Greek letters, is assigned to histidine; the Greek letters π and τ are used to designate the nitrogen atoms of the ring near to and far from the side chain, respectively.


β
α
CH2-CH(NH2)-COOH
5
4
τ HN
N π
2

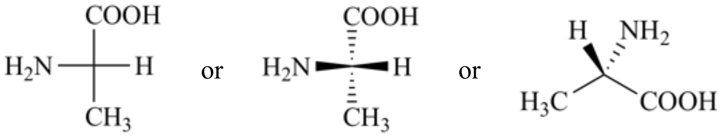
histidine

P-103.1.3 Configuration of α-amino carboxylic acids

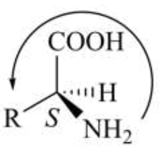
P-103.1.3.1 The stereodescriptors 'D' and 'L'

The absolute configuration at the α-carbon atom of the α-amino carboxylic acids is designated by the stereodescriptor 'D' or 'L' to indicate a formal relationship to 'D- or L-glyceraldehyde'. The stereodescriptor 'ξ' (Greek letter xi) indicates unknown configuration.

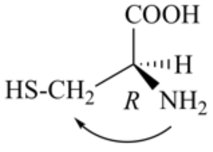
The structure of amino acids may be drawn to show configuration in several ways. A Fischer projection (see P-102.3.1) or a structural diagram including plain and wedged bonds (solid or hashed) may be used (see P-91.1), as drawn below for L-alanine:


COOH
H2N
H
CH3
or
COOH
H2N
H
CH3
or
H
NH2
H3C
COOH

The 'L' configuration corresponds to the '*S*' configuration of the CIP system, except that cysteine has the '*R*' configuration (and also cystine, see P-103.1.1.2).


COOH
H
R
S
NH2

L = *S*


COOH
H
HS-CH2
R
NH2

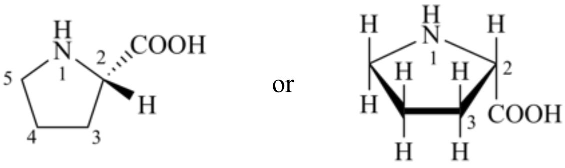
L = *R*, for cysteine

A mixture of equimolar amounts of ‘D’ and ‘L’ compounds is termed a ‘racemate’ and is designated by the stereodescriptor ‘DL’, for example ‘DL-leucine’. The stereodescriptor ‘DL’ is preferred to ‘*rac*’, i.e. *rac*-leucine.

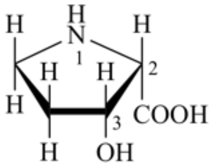
P-103.1.3.2 Configuration of chirality centers other than the α-carbon atom

P-103.1.3.2.1 Use of CIP stereodescriptors

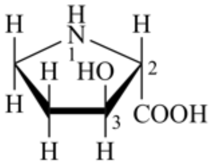
Stereodescriptors ‘*R*’ and ‘*S*’ are used for designating the configuration at centers other than the ‘α-C’ atom, while preserving stereodescriptors ‘D’ and ‘L’ for the ‘α-C’ atom to maintain homogeneity of stereodescriptors in peptides (see P-103.3.4). The use of stereodescriptors is exemplified here by the hydroxy prolines; for these compounds it is also acceptable to use the stereodescriptors *cis* and *trans* in the specialized nomenclature of amino acids and in general nomenclature.


H
N
1
2
COOH
5
H
4
3
or
H
H
N
H
1
H
H
2
H
3
COOH
H
H

L-proline
(2*S*)-proline


H
H
N
H
1
H
H
2
H
3
COOH
H
OH

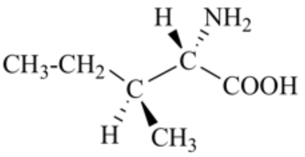
(3*R*)-3-hydroxy-L-proline
(2*S*,3*R*)-3-hydroxyproline
cis-3-hydroxy-L-proline


H
H
N
H
1
H
HO
2
H
3
COOH
H
H

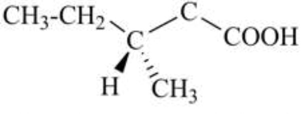
(3*S*)-3-hydroxy-L-proline
(2*S*,3*S*)-3-hydroxyproline
trans-3-hydroxy-L-proline

P-103.1.3.2.2 Use of the prefix ‘allo’

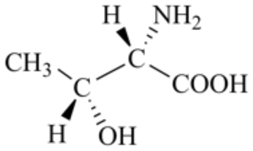
The prefix ‘allo’ is used to modify the retained names ‘isoleucine’ and ‘threonine’ when the configuration at ‘C-3’ has been inverted. The symbols are modified to ‘aIle’ and ‘aThr’, respectively.


H
NH2
CH3-CH2
C
C
COOH
H
CH3

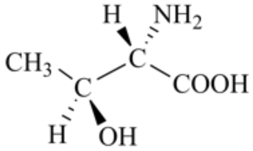
L-isoleucine (symbols ‘Ile’, ‘ I’)
(2*S*,3*S*)-2-amino-3-methylpentanoic acid


H
NH2
CH3-CH2
C
C
COOH
H
CH3

L-alloisoleucine (symbol ‘aIle’)
(2*S*,3*R*)-2-amino-3-methylpentanoic acid



L-threonine (symbols ‘Thr’,‘T’)
(2*S*,3*R*)-2-amino-3-hydroxybutanoic acid



L-allothreonine (symbol ‘aThr’)
(2*S*,3*S*)-2-amino-3-hydroxybutanoic acid

P-103.2 DERIVATIVES OF AMINO ACIDS

Retained names are used to generate names of salts, esters and acyl groups, and those of derivatives formed by substitution on carbon and nitrogen atoms or functionalization on oxygen and sulfur atoms.

The carboxy group, –COOH, can be transformed into various characteristic groups such as a hydroxymethyl group, –CH_2-OH, or an aldehyde group, –CHO. Some names derived from retained amino acid names are recommended to be used for naming amides, alcohols, aldehydes, and even ketones, in the context of peptide and protein nomenclature.

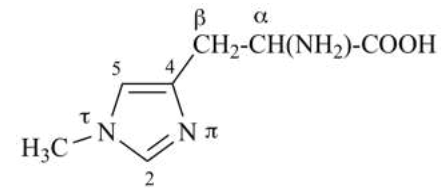
P-103.2.1 System for denoting locants
P-103.2.2 Names of substituent groups
P-103.2.3 Derivatives formed by substitution
P-103.2.4 Ionization of characteristic groups
P-103.2.5 Acyl groups
P-103.2.6 Esters
P-103.2.7 Amides, anilides, hydrazides, and other nitrogeneous analogues
P-103.2.8 Alcohols, aldehydes, ketones and nitriles

P-103.2.1 System for denoting locants

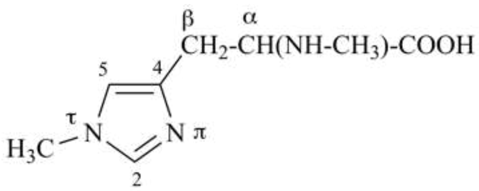
It is recommended to use ‘*N*’, ‘*O*’ and ‘*S*’ locants with the numerical locant of the attached carbon atom as a superscript to describe substitution on a nitrogen, oxygen, or sulfur atom when more than one is present. Locants ‘N^{2}’ and ‘N^{6}’ are recommended for lysine,‘N^{α}’,‘N^{δ}’ and ‘N^{ω}’ for arginine, ‘N^{2}’ and ‘N^{5}’ for glutamine,‘N^{2}’ and ‘N^{4}’ for asparagine, ‘N^{α}’, ‘N^{π}’ and ‘N^{τ}’ for histidine, according to the numbering of the corresponding α-amino acids described in P-103.1.2. When only one nitrogen is present, the locant ‘*N*’ is recommended; the numerical locant being omitted, even when other locants are present in the name.

When two identical substituent groups are present one letter locant is used between the multiplicative prefix and the name of the substituent group.

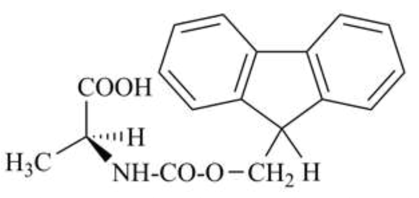
Examples:



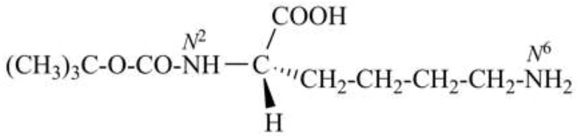
N^{τ}-methyl-L-histidine



N^{α},N^{τ}-dimethyl-L-histidine

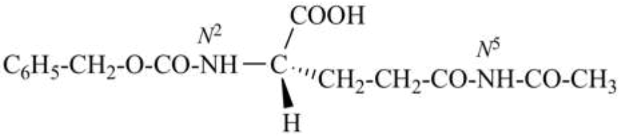


N-[(9*H*-fluoren-9-ylmethoxy)carbonyl]-L-alanine



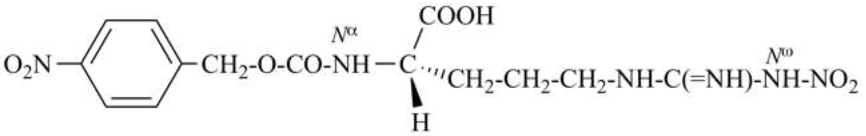
$(CH_3)_3C\text{-}O\text{-}CO\text{-}\overset{N^2}{NH}-\underset{H}{\overset{COOH}{C}}\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}\overset{N^6}{NH_2}$

N^2-(*tert*-butoxycarbonyl)-L-lysine



$C_6H_5\text{-}CH_2\text{-}O\text{-}CO\text{-}\overset{N^2}{NH}-\underset{H}{\overset{COOH}{C}}\text{-}CH_2\text{-}CH_2\text{-}CO\text{-}\overset{N^5}{NH}\text{-}CO\text{-}CH_3$

N^5-acetyl-N^2-[(benzyloxy)carbonyl]-L-glutamine



N^α-{[(4-nitrobenzyl)oxy]carbonyl}-N^ω-nitro-L-arginine

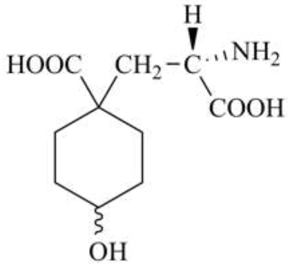
P-103.2.2 Names of substituent groups

When α-amino carboxylic acids must be cited as substituent groups in the presence of characteristic groups having seniority for citation as suffix, prefixes are formed according to the following principles.

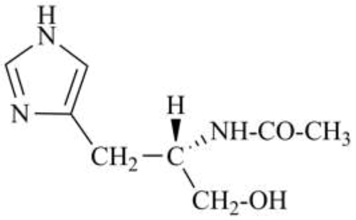
P-103.2.2.1 Substituent groups with the free valence on a carbon atom

Substituent groups with the free valence on a carbon atom of an α-amino carboxylic acid are formed according to the rules, principles and conventions of substitutive nomenclature as given in the previous chapters of these recommendations.

Examples:



1-[(2*S*)-2-amino-2-carboxyethyl]-4ξ-hydroxycyclohexane-1-carboxylic acid



N-[(2*S*)-1-hydroxy-3-(1*H*-imidazol-4-yl)propan-2-yl]acetamide

P-103.2.2.2 Substituent groups with the free valence on a nitrogen atom

Substituent groups with the free valence on a nitrogen atom of an α-amino carboxylic acid formed by the removal of a hydrogen atom from the amino group of an amino acid may be named by changing the ending ‘e’ of the name of the α-amino acid into ‘o’, by adding the letter ‘o’ to tryptophan and by constructing the names asparto and glutamo, from aspartic acid and glutamic acid, respectively.

Example:

$-HN\text{-}CH_2\text{-}COOH$

glycino

(carboxymethyl)amino

When there is more than one nitrogen atom in the amino acid, the use of a locant of the form ‘N^x’ is recommended.

Examples:

–HN-$[CH_2]_4$-CH(NH_2)-COOH
N^6-lysino
(5-amino-5-carboxypentyl)amino

–HN-C(=NH)-NH-$[CH_2]_3$-CH(NH_2)-COOH
N^{ω}-arginino
N′-[(4-amino-4-carboxybutyl)amino]carbamimidamido

–HN-CO-$[CH_2]_2$-CH(NH_2)-COOH
N^5-glutamino
4-amino-4-carboxybutanamido

P-103.2.2.3 Substituent groups with the free valence on an oxygen or sulfur atom formed by subtraction of a hydrogen atom from an oxygen or sulfur atom may also be named by changing the final letter ‘e’, when appropriate, of the name of the α-amino acid to ‘*x*-yl’, *x* being the locant of the atom from which the hydrogen atom has been subtracted, for example cystein-*S*-yl, threonin-*O*-yl.

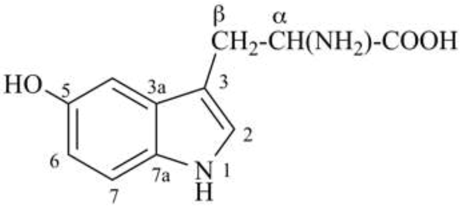
Example:

–S-CH_2-CH(NH_2)-COOH
cystein-*S*-yl
(2-amino-2-carboxyethyl)sulfanyl

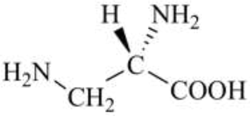
P-103.2.3 Derivatives formed by substitution

Retained names are used to indicate carbon, nitrogen, oxygen and sulfur substitution. Substitution on carbon atoms follows the principles, rules and conventions of substitutive nomenclature. Numerical locants and locants ‘*N*’, ‘*O*’, and ‘*S*’ indicate the location of the substitution on nitrogen, oxygen, or sulfur atoms. For lysine, locants ‘N^2’ and ‘N^6’ are used to denote the two amino groups located at positions ‘2’ and ‘6’, respectively.

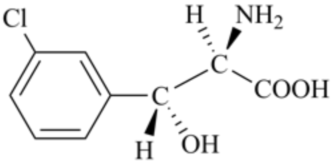
Examples:



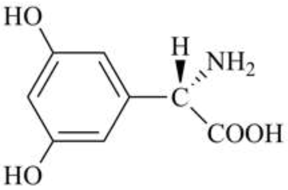
5-hydroxytryptophan



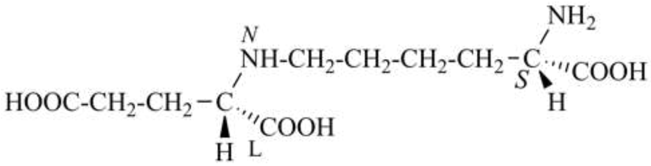
3-amino-L-alanine
(2*S*)-2,3-diaminopropanoic acid
L-2,3-diaminopropanoic acid
(2*S*)-2-amino-β-alanine (see ref. 18)



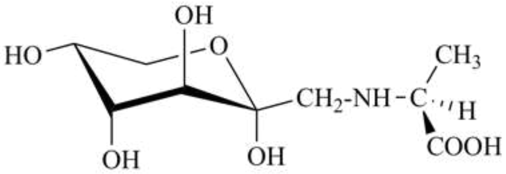
(2*R*,3*R*)-2-amino-3-(3-chlorophenyl)-3-hydroxypropanoic acid
(β*R*)-3-chloro-β-hydroxy-D-phenylalanine



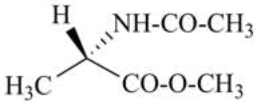
(2*S*)-2-amino-2-(3,5-dihydroxyphenyl)acetic acid
2-(3,5-dihydroxyphenyl)-L-glycine



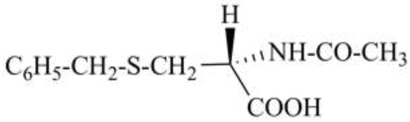
N-[(5*S*)-5-amino-5-carboxypentyl]-L-glutamic acid



N-(1-deoxy-α-D-fructopyranos-1-yl)-L-alanine



methyl *N*-acetyl-L-alaninate



S-benzyl-L-cysteine

$(HO)_2N-CH_2-COOH$
N,*N*-dihydroxyglycine

$(HO)_2N-CH(NH_2)-COOCH_3$
N-(1-amino-2-methoxy-2-oxoethyl)azonous acid
[an acid, azonous acid for $(HO)_2NH$, is senior to an ester; see P-67.1.1.1]

P-103.2.4 Ionization of characteristic groups

P-103.2.4.1 The predominant form of a monoamino monocarboxylic acid in a neutral solution (pH 7) is $R-CH(NH_3^+)-COO^-$ rather than $R-CH(NH_2)-COOH$. It is nevertheless convenient to draw the conventional form as in Tables 10.4 and 10.5 and to name the amino acid alanine as 2-aminopropanoic acid rather than as 2-azaniumylpropanoate, 2-ammoniumylpropanoate or 2-ammoniopropanoate as in Chapter P-7 (P-74.1.3).

This is particularly so for representing the isoelectric forms of amino acids that contain other ionizing groups, such as a solution of lysine, which would contain appreciable amounts of both $NH_3^+-[CH_2]_4-CH(NH_2)-COO^-$ and $NH_2-[CH_2]_4-CH(NH_3^+)-COO^-$.

P-103.2.4.2 When it is desirable to mention or stress the ionic nature of an amino acid, cations or anions derived from a monoamino monocarboxylic acid may be indicated as follows (in indicating an anion the ending 'ate' replaces 'ic acid' or the final 'e' of the trivial name, or is added to the name tryptophan):

Examples:

$H_2N-CH_2-COO^-$
glycinate
glycine anion

$NH_3^+-CH_2-COOH$
glycinium
glycine cation

P-103.2.4.3 Further forms are required for amino acids that contain two amino groups or two carboxylic groups.

P-103.2.4.3.1 The singly charged anions of aspartic and glutamic acids (strictly each has one positive charge and two negative charges, but this nomenclature refers to net charge) and may be distinguished from the doubly charged anions by placing the charge after the name or by stating the number of neutralizing cations.

Examples:

$^-OOC-CH_2-CH_2-CH(NH_2)-COO^-\ H^+$
glutamate(1–)
hydrogen glutamate
glutamic acid monoanion

$^{-}OOC-CH_2-CH_2-CH(NH_2)-COO^{-}\ Na^{+}\ H^{+}$
sodium glutamate
sodium hydrogen glutamate
monosodium glutamate

$^{-}OOC-CH_2-CH_2-CH(NH_2)-COO^{-}$
glutamate(2–)
glutamic acid dianion
glutamate (unqualified, the name 'glutamate' means the dianion)

$^{-}OOC-CH_2-CH_2-CH(NH_2)-COO^{-}\ 2Na^{+}$
disodium glutamate

P-103.2.4.3.2 The singly charged cations of arginine, histidine, and lysine (strictly each has two positive charges and one negative charge, but this nomenclature refers to net charge) may be distinguished from the doubly charged cations by placing the charge after the name, by the phrase 'monocation', or by stating the number of neutralizing anions. The location of the charge may be specified by a superscripted '*N*' locant placed before the 'ium' ending.

Examples:

$NH_2-[CH_2]_4-CH(NH_3^{+})-COOH$
lysinium(1+)
lysine monocation
lysin-*N*^{2}-ium

$NH_2-[CH_2]_4-CH(NH_3^{+})-COOH\ Cl^{-}$
lysinium(1+) chloride
lysine monohydrochloride
lysin-*N*^{2}-ium chloride

$NH_3^{+}-[CH_2]_4-CH(NH_3^{+})-COOH$
lysinium(2+)
lysine dication
lysine-*N*^{2},*N*^{6}-diium

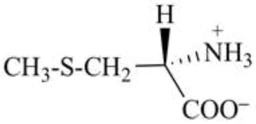
P-103.2.4.4 Zwitterionic amino acids are named in two ways:

(1) by prefixing the name of the cationic substituent group into that of the anionic parent (see P-74.1.3) and using CIP stereodescriptors to describe the configuration;

(2) by adding the term 'zwitterion' to the name of the amino acid.

Examples:

$H_3N^{+}-CH_2-COO^{-}$
azaniumylacetate
glycine zwitterion



(2*S*)-2-azaniumyl-3-(methylsulfanyl)propanoate
S-methyl-L-cysteine zwitterion

P-103.2.5 Acyl groups

Acyl groups derived from organic acids, for example $H_2N-CHR-CO–$, are named by changing the ending 'ine' (or 'an' in tryptophan) into 'yl', for example alanyl, valyl, tryptophyl. 'Cysteinyl' is used instead of 'cysteyl'; 'cystyl' is derived from 'cystine' (see P-103.1.1.2).

The following names are used to name the acyl groups derived from dicarboxylic amino acids and their corresponding amides:

$HOOC-CH_2-CH(NH_2)-CO–$
α-aspartyl
aspart-1-yl

$–CO-CH_2-CH(NH_2)-COOH$
β-aspartyl
aspart-4-yl

$-CO-CH_2-CH(NH_2)-CO-$
aspartoyl

$HOOC-CH_2-CH_2-CH(NH_2)-CO-$
α-glutamyl
glutam-1-yl

$-CO-CH_2-CH_2-CH(NH_2)-COOH$
γ-glutamyl
glutam-5-yl

$-CO-CH_2-CH_2-CH(NH_2)-CO-$
glutamoyl

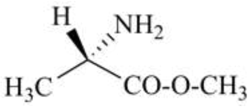
$H_2N-CO-CH_2-CH(NH_2)-CO-$
asparaginyl

$H_2N-CO-CH_2-CH_2-CH(NH_2)-CO-$
glutaminyl

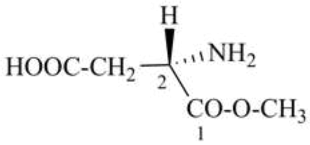
P-103.2.6 Esters

Esters of amino acids, $R-CO-OR'$, are formed by the general method using the ‘ate’ ending obtained by replacing the ‘ic acid’ ending or the final letter ‘e’ of the retained name (or adding the ending ‘ate’ to the name tryptophan) and the name of the substituent group R′.

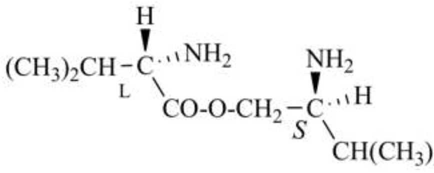
Examples:



methyl L-alaninate
L-alanine methyl ester



1-methyl L-aspartate



(2*S*)-2-amino-3-methylbutyl L-valinate

P-103.2.7 Amides, anilides, hydrazides, and other nitrogenous analogues

Amides, anilides, hydrazides, and other nitrogenous analogues derivatives derived from amino acids are named systematically.

Names of amides derived from amino acids are formed by changing the final letter ‘e’ in the names of amino acids, when appropriate, into ‘amide’ or adding the term ‘amide’ to the name tryptophan.

Examples:

$H_2N-CH_2-CO-NH_2$
2-aminoacetamide
glycinamide

The 4-amide of aspartic acid has its own name, asparagine, and the 5-amide of glutamic acid is glutamine (see Table 10.4). Their 1-amides are named as follows:

$H_2N\text{-}CO\text{-}CH_2\text{-}CH(NH_2)\text{-}CO\text{-}NH_2$
2-aminobutanediamide
asparaginamide

$H_2N\text{-}CO\text{-}CH_2\text{-}CH_2\text{-}CH(NH_2)\text{-}CO\text{-}NH_2$
2-aminopentanediamide
glutaminamide

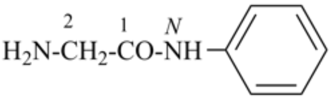
The 1-amides of aspartic acid and glutamic acid are named as follows:

$HO\text{-}CO\text{-}CH_2\text{-}CH(NH_2)\text{-}CO\text{-}NH_2$
3,4-diamino-4-oxobutanoic acid
aspartic 1-amide

$HO\text{-}CO\text{-}CH_2\text{-}CH_2\text{-}CH(NH_2)\text{-}CO\text{-}NH_2$
4,5-diamino-5-oxopentanoic acid
glutamic 1-amide

Names of anilides are formed by *N*-substitution of the amide group by the phenyl group or a substituted phenyl group. The ending 'anilide', in place of 'amide', may also be used.

Example:



2-amino-N^1-phenylacetamide
glycinanilide

Substitution on nitrogen atoms in amides of amino acids is expressed systematically by the methods described for amides (P-66.1.1.3) and amines (P-62.2.2.1).

Examples:

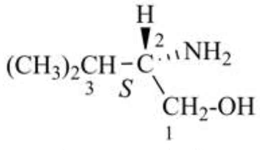
$CH_3\text{-}NH\text{-}CH_2\text{-}CO\text{-}NH\text{-}CH_2\text{-}CH_3$
N-ethyl-2-(methylamino)acetamide

$CH_3\text{-}CO\text{-}NH\text{-}CH_2\text{-}CO\text{-}NH_2$
2-(acetylamino)acetamide
2-acetamidoacetamide
N^2-acetylglycinamide

P-103.2.8 Alcohols, aldehydes, ketones, and nitriles

Alcohols, aldehydes, ketones and nitriles corresponding to amino acids with retained trivial names are named systematically by using the principles, rules and conventions of substitutive nomenclature. The endings 'ol', 'al', 'one' and 'onitrile' are added to retained names, with elision of the final letter 'e' and may be used to designate a change in the characteristic group of an amino acid. Ketones must be named using systematic IUPAC substitutive nomenclature with '*R*' and '*S*' stereodescriptors when needed.

Examples:



(2*S*)-2-amino-3-methylbutan-1-ol
L-valinol

$(CH_3)_2CH\text{-}CH_2\text{-}CH(NH_2)\text{-}CHO$
2-amino-4-methylpentanal
leucinal

$H_2N\text{-}CH_2\text{-}CO\text{-}CH_2Cl$
1-amino-3-chloropropan-2-one

$H_2N\text{-}CH_2\text{-}C{\equiv}N$
aminoacetonitrile
glycinonitrile

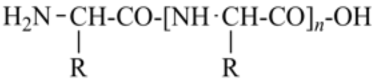
P-103.3 NOMENCLATURE OF PEPTIDES

Nomenclature of peptides is highly specialized and well documented in ref. 18. Nomenclature of cyclic peptides is under study by the IUPAC Chemical Nomenclature and Structure Representation Division.

P-103.3.1 Definitions
P-103.3.2 Names of peptides
P-103.3.3 Symbols of peptides
P-103.3.4 Indication of configuration in peptides
P-103.3.5 Modification of named peptides
P-103.3.6 Cyclic peptides

P-103.3.1 Definitions

Peptides are amides derived from two or more amino carboxylic acid molecules (the same or different) by formation of a covalent bond from the carbonyl carbon of one to the nitrogen atom of another with formal loss of water. The term is usually applied to structures formed from α-amino carboxylic acids, but it includes those derived from any amino carboxylic acid. In the following example, 'R' may be any organyl group, commonly but not necessarily one found in 'common' amino acids (see Table 10.4):



$$H_2N-\underset{\displaystyle R}{\underset{|}{C}H}-CO-[NH\cdot\underset{\displaystyle R}{\underset{|}{C}H}-CO]_n-OH$$

The amide bonds in peptides are called 'peptide bonds'. Peptides bonds formed between 'C-1' of one amino acid and 'N-2' of another amino acid are called 'eupeptide bonds'. Those formed between an amino group of one amino acid and a carboxy group of another amino acid, which are not 'eupeptide' bonds, are called 'isopeptide bonds'.

P-103.3.2 Names of peptides

To name peptides, the names of acyl groups ending in 'yl' (see P-103.2.5) are used. Thus if the amino acids glycine, H_2N-CH_2-COOH, and alanine, $H_2N-CH(CH_3)-COOH$, condense so that glycine acylates alanine, the dipeptide formed, $H_2N-CH_2-CO-NH-CH(CH_3)-COOH$, is named glycylalanine. If they condense in the reverse order, the product $H_2N-CH(CH_3)-CO-NH-CH_2-COOH$ is named alanylglycine. Higher peptides are named similarly, e.g. alanylleucyltryptophan.

P-103.3.3 Symbols of peptides

The peptide glycylglycylglycine is symbolized as Gly-Gly-Gly. This involves modifying the symbols Gly for glycine, H_2N-CH_2-COOH, by adding hyphens to it, in three ways:

(a) Gly- = $H_2N-CH_2-CO–$

(b) -Gly = $–HN-CH_2-COOH$

(c) -Gly- = $–HN-CH_2-CO–$

Thus the hyphen, which represents the peptide bond, removes an –OH group from the –COOH group of the amino acid when written on the right of the symbol, and a hydrogen atom, when written on the left of the symbol.

P-103.3.4 Indication of configuration in peptides

The stereodescriptor 'L' is not indicated in the names nor in the symbolic representation of peptides composed of amino acids listed in Table 10.4. In contrast, the stereodescriptor 'D' is indicated at the front of the acyl group or name of each component having that configuration.

Example:

Leu-D-Glu-L-aThr-D-Val-Leu
(the symbol aThr is for allothreonine);
L-leucyl-D-glutamyl-L-allothreonyl-D-valyl-L-leucine

The symbol 'DL' is used to indicate a racemic mixture when one chirality center is present as indicated in P-103.1.3.1 but is not allowed in peptides, as its presence indicates the presence of diastereoisomers in unknown proportions. The italicized prefix *ambo* is used to indicate that both stereoisomers are present, for example, the result of the acylation of L-leucine by DL-alanine is *ambo*-alanylleucine or *ambo*-Ala-Leu. A residue of unknown configuration is indicated by the prefix ξ (Greek letter xi). The enantiomer of a named peptide is specified by the prefix *ent* (for *enantio*, see P-101.8.1), giving *ent*-bradykinin from bradykinin.

P-103.3.5 Modification of named peptides

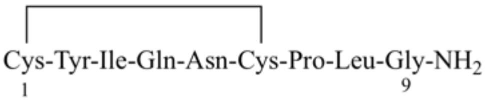
It is often convenient to specify the structure of a peptide by reference to a named sequence to which it is a variant. The recommendations that follow allow this, but they apply only to modification of the sequence involving normal amide links between residues. The retained names angiotensin II, bradikinin, oxytocin, and insulin (human) are used to illustrate these recommendations.

$\overset{1}{\text{Asp}}$-Arg-Val-Tyr-Xaa-His-Pro-$\overset{8}{\text{Phe}}$

angiotensin II

Arg-Pro-Pro-Gly-Phe-Ser-Pro-Phe-Arg

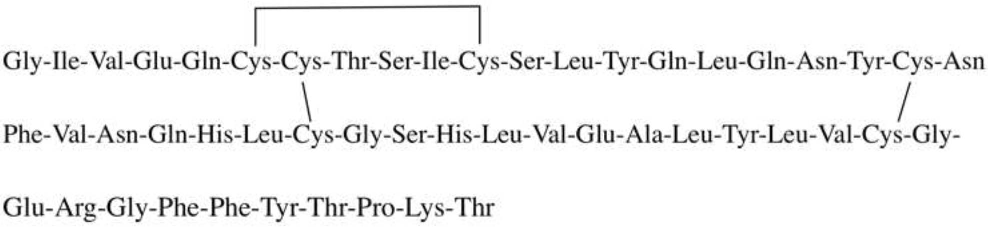
bradykinin


Cys-Tyr-Ile-Gln-Asn-Cys-Pro-Leu-Gly-NH2
1
9

oxytocin

Specification of a sequence may require the species as well as the peptide to be named (see insulin below). If so, the name of the species must be attached, in parentheses, to the peptide whenever a modifying prefix is present.

Chain A


Gly-Ile-Val-Glu-Gln-Cys-Cys-Thr-Ser-Ile-Cys-Ser-Leu-Tyr-Gln-Leu-Gln-Asn-Tyr-Cys-Asn
Phe-Val-Asn-Gln-His-Leu-Cys-Gly-Ser-His-Leu-Val-Glu-Ala-Leu-Tyr-Leu-Val-Cys-Gly-
Glu-Arg-Gly-Phe-Phe-Tyr-Thr-Pro-Lys-Thr

Chain B

insulin (human)

P-103.3.5.1 Replacement of residues
P-103.3.5.2 Extension of the peptide chain
P-103.3.5.3 Insertion of residues
P-103.3.5.4 Removal of residues

P-103.3.5.1 Replacement of residues

In a peptide of trivial name bradykinin, if the *q*th amino acid residue, starting from the ‘N-terminal’ end of the chain is replaced by the amino acid ‘Xaa’, the name of the modified peptide is [*q*-aminoacid]bradikinin and the abbreviated form is [Xaa^{q}]bradykinin. In a full name, the replacement amino acid is designated by its residue name, not the name of its acyl group (e.g. alanine, not alanyl). In the abbreviated form, the amino acid residues are designated by three letter symbols. In the abbreviated form, the position of replacement is indicated by a superscript.

Examples:

$\overset{1}{\text{Arg}}$-$\overset{2}{\text{Lys}}$-Pro-Gly-Phe-Ser-Pro-Phe-$\overset{9}{\text{Arg}}$

[2-lysine]bradykinin

[Lys^{2}]bradykinin

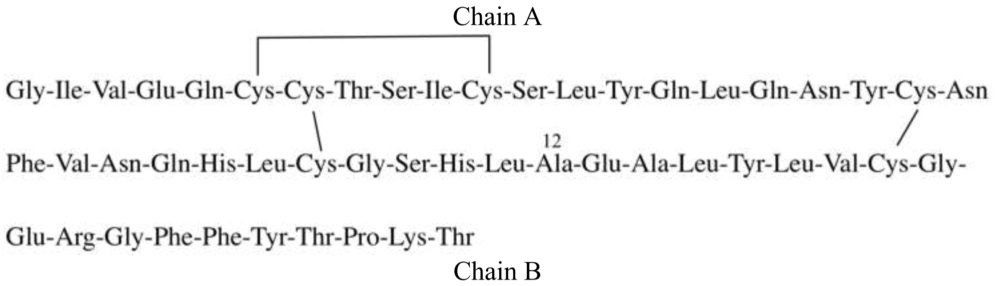
$\overset{1}{\text{Asp}}$-Arg-Val-Tyr-$\overset{5}{\text{Ile}}$-His-$\overset{7}{\text{Ala}}$-$\overset{8}{\text{Phe}}$

[5-isoleucine,7-alanine]angiotensin II

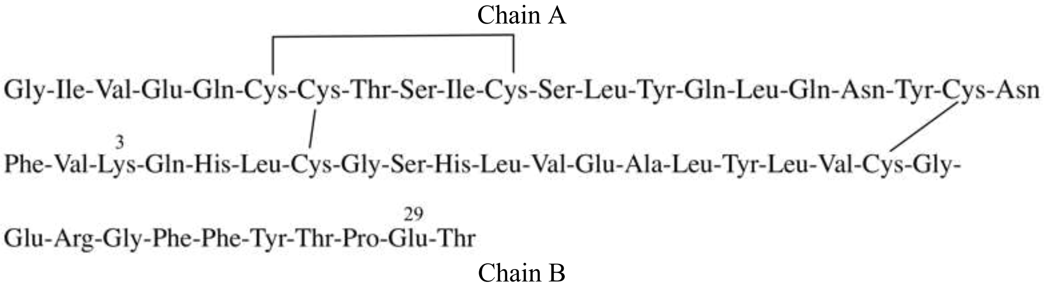
[Ile^{5},Ala^{7}]angiotensin II

P-103.3.5.1.1 The specification of a sequence requires the species as well as the peptide to be named. If so, the name of the species must be attached, in parentheses, to the name of the peptide whenever a modifying prefix is present.

Examples:


Chain A
Gly-Ile-Val-Glu-Gln-Cys-Cys-Thr-Ser-Ile-Cys-Ser-Leu-Tyr-Gln-Leu-Gln-Asn-Tyr-Cys-Asn
12
Phe-Val-Asn-Gln-His-Leu-Cys-Gly-Ser-His-Leu-Ala-Glu-Ala-Leu-Tyr-Leu-Val-Cys-Gly-
Glu-Arg-Gly-Phe-Phe-Tyr-Thr-Pro-Lys-Thr
Chain B

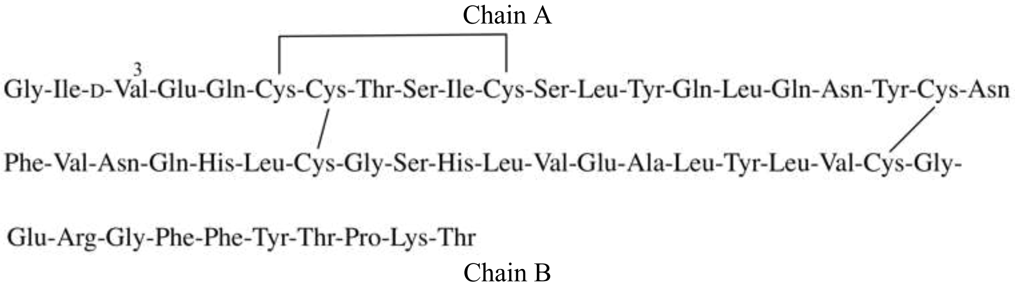
[Ala^{B12}]insulin (human)


Chain A
Gly-Ile-Val-Glu-Gln-Cys-Cys-Thr-Ser-Ile-Cys-Ser-Leu-Tyr-Gln-Leu-Gln-Asn-Tyr-Cys-Asn
3
Phe-Val-Lys-Gln-His-Leu-Cys-Gly-Ser-His-Leu-Val-Glu-Ala-Leu-Tyr-Leu-Val-Cys-Gly-
29
Glu-Arg-Gly-Phe-Phe-Tyr-Thr-Pro-Glu-Thr
Chain B

[B3-lysine,B29-glutamic acid]insulin (human)

P-103.3.5.1.2 The replacement of an amino acid residue by its enantiomer is expressed as follows. The replacement of L-proline in position 3 by D-proline results in [3-D-proline]bradykinin with the abbreviation [D-Pro^3]bradykinin. A mixture of this with bradykinin gives [3-*ambo*-proline]bradykinin or [*ambo*-Pro^3]bradykinin.

Example:


Chain A
3
Gly-Ile-D-Val-Glu-Gln-Cys-Cys-Thr-Ser-Ile-Cys-Ser-Leu-Tyr-Gln-Leu-Gln-Asn-Tyr-Cys-Asn
Phe-Val-Asn-Gln-His-Leu-Cys-Gly-Ser-His-Leu-Val-Glu-Ala-Leu-Tyr-Leu-Val-Cys-Gly-
Glu-Arg-Gly-Phe-Phe-Tyr-Thr-Pro-Lys-Thr
Chain B

[D-Val^{A3}]insulin (human)

P-103.3.5.2 Extension of the peptide chain

The compounds obtained by the extension of a peptide at either the N-terminus or the C-terminus are designated by the kind of names and abbreviations shown below.

P-103.3.5.2.1 Extension at the ‘N-terminus’

Examples:

$\overset{1}{\text{Val}}$-Arg-Pro-Pro-Gly-Phe-Ser-Pro-Phe-$\overset{9}{\text{Arg}}$

valylbradykinin
Val-bradykinin

Val-Gly-$\overset{1}{\text{Arg}}$-Pro-Pro-Gly-Phe-Ser-Pro-Phe-$\overset{9}{\text{Arg}}$

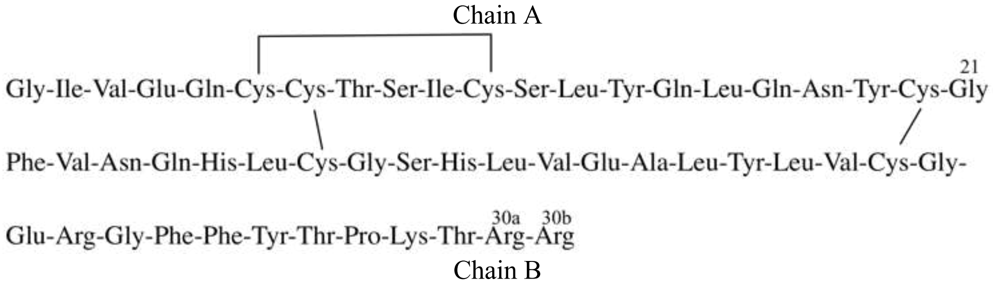
valylglycylbradykinin
Val-Gly-bradykinin

P-103.3.5.2.2 Extension at the ‘C-terminus’

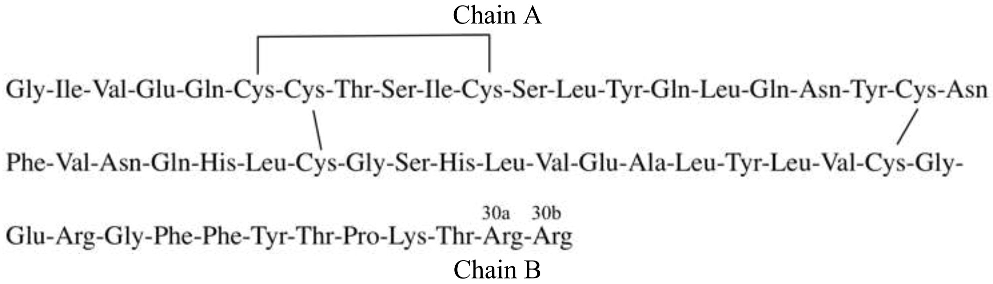
Examples:

$\overset{1}{\text{Arg}}$-Pro-Pro-Gly-Phe-Ser-Pro-Phe-$\overset{9}{\text{Arg}}$-Leu

bradykininylleucine
bradykininyl-Leu



insulin-B30-yl-L-argininyl-L-arginine (human)

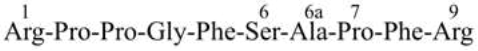


[A21-glycine]insulin-B30-yl-L-argininyl-L-arginine (human)
(this insulin is modified by replacement in Chain A and extension at the C-terminus in Chain B)

P-103.3.5.3 Insertion of residues

In peptide nomenclature, the prefix ‘endo’ (nonitalic) is used to denote the insertion of an amino acid residue in a well identified position in the peptide. For example, the name endo-6a-alanine-bradykinin, or [endo-Ala^{6a}]bradykinin, means that the amino acid residue ‘alanyl’ has been inserted between the positions 6 and 7 in the structure of bradykinin. The prefix ‘endo’ is not to be confused with the recommended stereodescriptor ‘*endo*’ (written in italics) described in P-93.5.2.2.1.

Example:

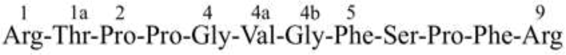


$\overset{1}{\text{Arg}}\text{-Pro-Pro-Gly-Phe-}\overset{6}{\text{Ser}}\text{-}\overset{6a}{\text{Ala}}\text{-}\overset{7}{\text{Pro}}\text{-Phe-}\overset{9}{\text{Arg}}$

endo-6a-alanine-bradykinin
[endo-Ala^{6a}]bradykinin

Multiple insertions, and insertion of a maximum of two residues, together in the same place in the chain are shown by a logical extension of this recommendation. Thus the insertion into the peptide bradykinin of threonine between residues 1 and 2, and of valine and glycine (in that order) between residues 4 and 5 is shown by the name ‘endo-1a-threonine,4a-valine,4b-glycine-bradykinin’ or ‘endo-Thr^{1a},Val^{4a},Gly^{4b}-bradykinin’.

Example:



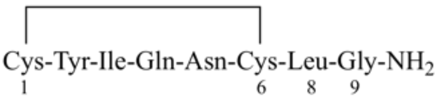
$\overset{1}{\text{Arg}}\text{-}\overset{1a}{\text{Thr}}\text{-}\overset{2}{\text{Pro}}\text{-Pro-}\overset{4}{\text{Gly}}\text{-}\overset{4a}{\text{Val}}\text{-}\overset{4b}{\text{Gly}}\text{-}\overset{5}{\text{Phe}}\text{-Ser-Pro-Phe-}\overset{9}{\text{Arg}}$

endo-1a-threonine,4a-valine,4b-glycine-bradykinin
endo-Thr^{1a},Val^{4a},Gly^{4b}-bradykinin

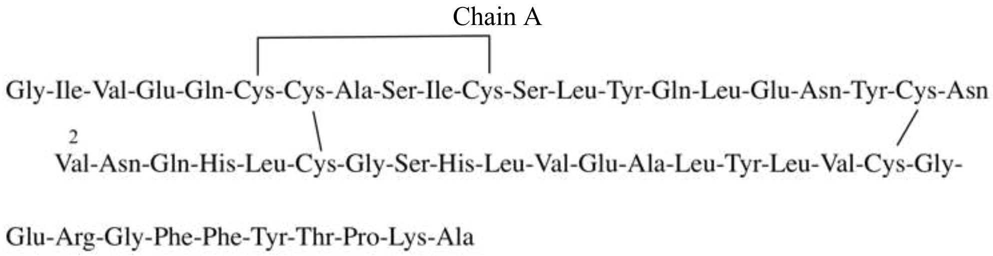
P-103.3.5.4 Removal of residues

The subtractive prefix ‘des’, in peptide nomenclature, is used to denote the removal of an amino acid residue from any position in a peptide structure. For example, the name des-8-phenylalanine-bradykinin means that the amino-acid residue ‘phenylalanyl’, located in position 8 of the peptide bradykinin, has been removed; or in the abbreviated form des-Phe^8-bradykinin. In the modification of parent structures described in Section P-101, the prefix ‘des’ is used to indicate the removal of a terminal ring in steroids with the addition of the appropriate number of hydrogen atoms at each junction with the adjacent ring (see P-101.3.6).

Examples:



des-7-proline-oxytocin
des-Pro^7-oxytocin


Chain A
Gly-Ile-Val-Glu-Gln-Cys-Cys-Ala-Ser-Ile-Cys-Ser-Leu-Tyr-Gln-Leu-Glu-Asn-Tyr-Cys-Asn
2
Val-Asn-Gln-His-Leu-Cys-Gly-Ser-His-Leu-Val-Glu-Ala-Leu-Tyr-Leu-Val-Cys-Gly-
Glu-Arg-Gly-Phe-Phe-Tyr-Thr-Pro-Lys-Ala

Chain B
des-B1-phenylalanine-insulin (cattle)
des-Phe^{B1}-insulin (cattle)

P-103.3.6 Cyclic peptides

Cyclic peptides include rings generated from a peptide (acyclic peptide) by formation of a peptide or ester bond, by a disulfide link, or by a new carbon-carbon, carbon-nitrogen, carbon-oxygen, or carbon-sulfur bond (excluding esters and amides). Cyclic peptides in which the ring consists entirely of amino acid residues with eupeptide bonds are called ‘homodetic cyclic peptides’. Those formed of eupeptide and isopeptide bonds are called ‘heterodetic cyclic peptides’. This aspect of peptide nomenclature is under study by the IUPAC Chemical Nomenclature and Structure Representation Division.

P-104 CYCLITOLS

P-104.0 Introduction
P-104.1 Definitions
P-104.2 Name construction
P-104.3 Derivatives of cyclitols

P-104.0 INTRODUCTION

The nomenclature of cyclitols is described in the document entitled ‘Nomenclature of Cyclitols, Recommendations 1973’ (ref. 39).

P-104.1 DEFINITIONS

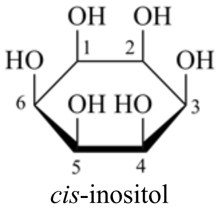
Cyclitols are cycloalkanes in which three or more ring atoms are each substituted with one hydroxy group. Inositols, cyclohexane-1,2,3,4,5,6-hexols, are a specific group of cyclitols.

Inositols have retained names and, together with their *O*-alkyl, *O*-aryl, alkanoate/carboxylate esters, and amino derivatives (where NH_2 replaces OH) employ the stereodescriptors ‘D’ and ‘L’ to describe configurations. Other names of cyclitols are systematic substitutive names whose configurations are described by CIP stereodescriptors.

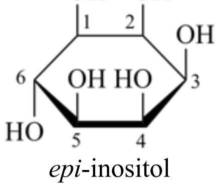
P-104.2 NAME CONSTRUCTION

Various methods are recommended for naming cyclitols.

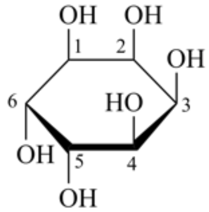
P-104.2.1 Stereoisomeric inositols are described by adding italicized prefixes at the front of the name ‘inositol’. Positional numbers described in the following method are indicated in parentheses. Names denoted by the prefixes are preferred.


OH
OH
HO
OH
1
2
6
OH HO
3
5
4

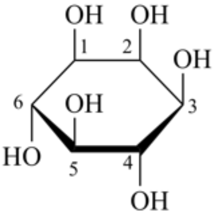
cis-inositol
(1,2,3,4,5,6/0)


OH
OH
OH
1
2
6
OH HO
3
HO
5
4

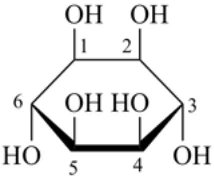
epi-inositol
(1,2,3,4,5/6-)



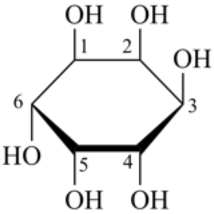
allo-inositol
(1,2,3,4/5,6-)



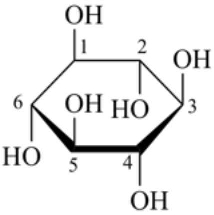
myo-inositol
(1,2,3,5/4,6-)



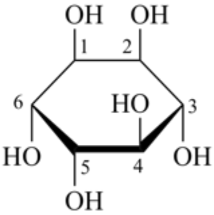
muco-inositol
(1,2,4,5/3,6-)



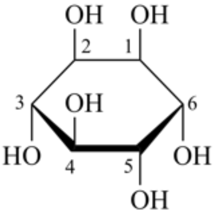
neo-inositol
(1,2,3/4,5,6-)



scyllo-inositol
(1,3,5/2,4,6-)



1L-*chiro*-inositol
(1,2,4/3,5,6-)
[formerly L-*chiro*-inositol or
(–)-inositol]

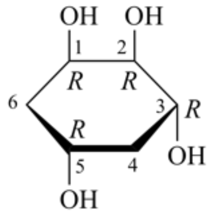


1D-*chiro*-inositol
(1,2,4/3,5,6-)
[formerly D-*chiro*-inositol or (+)-inositol]

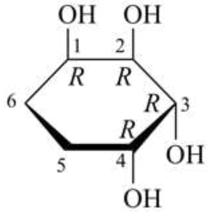
The absolute configuration of cyclitols is denoted by ‘D’ and ‘L’ and is determined in the following way. For the planar ring representation where the hydroxy group numbered ‘1’ is above the plane of the ring, the configuration ‘L’ corresponds to a clockwise numbering, and the configuration ‘D’ corresponds to an anticlockwise numbering, as illustrated by the two enantiomeric *chiro*-inositols above. The stereodescriptors ‘D’ and ‘L’ followed by a hyphen are placed before the name of the compound and are preceded by the locant of the defining center, i.e. ‘1’ as shown above.

P-104.2.2 Cyclitols, with the exception of inositols, are named systematically from cyclohexane as the parent using the CIP method and its Sequence Rules for describing stereoisomers. This method is preferred to the method of positional numbers described in P-104.2.3.

Examples:



(1*R*,2*R*,3*R*,5*R*)-cyclohexane-1,2,3,5-tetrol



(1*R*,2*R*,3*R*,4*R*)-cyclohexane-1,2,3,4-tetrol

P-104.2.3 Locants are assigned to hydroxy groups in cyclitols, and thus the direction of numbering is described, with reference to the steric relations and nature of the substituents attached to the ring. The substituents lying above the plane of the ring constitute a set, and those lying below another set. Lowest locants are related to one set of the substituents according to the following criteria, which are applied successively until a decision is reached:

(a) to the substituents considered as a numerical series, without regard to configuration;

(b) if one set of the substituents is more numerous than the other, to the more numerous;

(c) if the sets are equally numerous and one of them can be denoted by lower numbers, to that set;

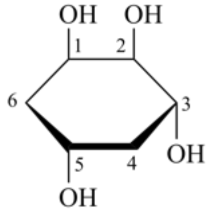
(d) to substituents other than unmodified hydroxy groups;

(e) to the substituent first cited in alphanumerical order;

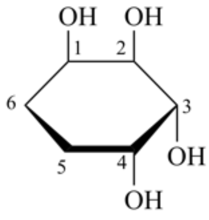
(f) to those designations that lead to an ‘L’ rather than a ‘D’ configuration, as determined by the method of P-104.2.1 above (applies to *meso* compounds only).

The positional numbers are described by a fractional expression in which the numerator is the set of substituents with the lowest locants, arranged in ascending order, and the denominator is the other set.

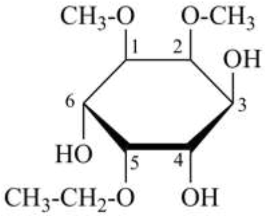
Examples:



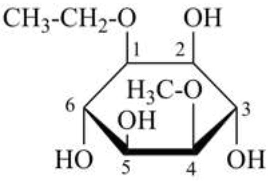
1L-1,2/3,5-cyclohexanetetrol [criteria (a) and (c)]
(1*R*,2*R*,3*R*,5*R*)-cyclohexane-1,2,3,5-tetrol



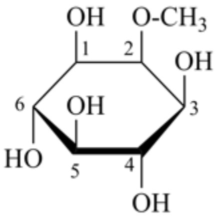
1L-1,2/3,4-cyclohexanetetrol [criterion (a)]
(1*R*,2*R*,3*R*,4*R*)-cyclohexane-1,2,3,4-tetrol


CH3-O
O-CH3
OH
1
2
3
6
HO
5
4
CH3-CH2-O
OH

1L-5-*O*-ethyl-1,2-di-*O*-methyl-*neo*-inositol [criterion (d)]


CH3-CH2-O
OH
1
2
H3C-O
6
OH
3
HO
5
4
OH

1L-1-*O*-ethyl-4-*O*-methyl-*muco*-inositol [criteria (d) and (e)]


OH
O-CH3
1
2
OH
6
OH
3
HO
5
4
OH

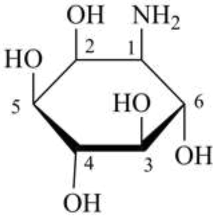
2-*O*-methyl-*myo*-inositol [criteria (b) and (f)]

P-104.3 DERIVATIVES OF CYCLITOLS

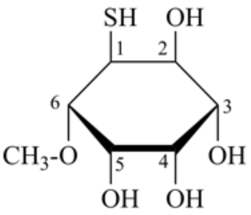
P-104.3.1 Derivatives of inositols

Inositols are modified in the same way as carbohydrates to generate names for derivatives. There is no limit to *O*-substitution by alkyl (aryl) groups (see P-102.5.6.1). Hydroxy groups can be exchanged for amino groups using the 'deoxy' operation (see P-102.5.4). When characteristic groups that are senior to hydroxy groups are put in the place of a hydroxy group, fully substitutive names must be constructed. However, esters are named as alkanoates/carboxylates. The numbering of the inositol remains unchanged and the configuration is expressed by an 'L' or 'D' stereodescriptor. Systematic names may have different numbering from the corresponding inositol name (see examples 2 and 5).

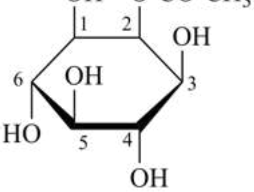
Examples:


OH
NH2
HO
2
1
5
HO
6
4
3
OH
OH

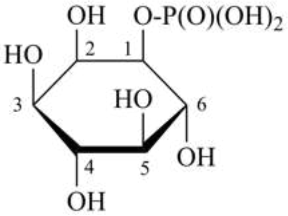
1D-1-amino-1-deoxy-*myo*-inositol


SH
OH
1
2
6
3
CH3-O
5
4
OH
OH
OH

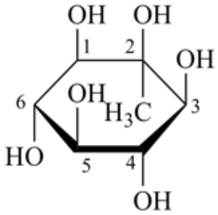
1L-1-deoxy-6-*O*-methyl-1-sulfanyl-*allo*-inositol
(not 1L-6-*O*-methyl-1-thio-*allo*-inositol)
(1*S*,2*R*,3*S*,4*S*,5*S*,6*S*)-5-methoxy-6-sulfanylcyclohexane-1,2,3,4-tetrol


OH
O-CO-CH3
1
2
OH
6
OH
3
HO
5
4
OH

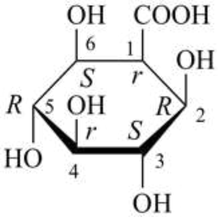
myo-inositol 2-acetate
(see P-102.5.6.1.1 for naming carbohydrate esters)



1D-*myo*-inositol 1-(dihydrogen phosphate)



2-*C*-methyl-*myo*-inositol
(1*s*,2*R*,3*S*,4*s*,5*R*,6*S*)-1-methylcyclohexane-1,2,3,4,5,6-hexol

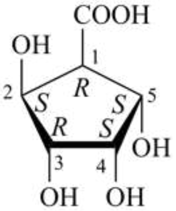


(1*r*,2*R*,3*S*,4*r*,5*R*,6*S*)-2,3,4,5,6-pentahydroxycyclohexane-1-carboxylic acid
(not 2-carboxy-2-deoxy-*myo*-inositol;
COOH is senior to OH)

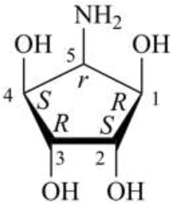
P-104.3.2 Derivatives of cyclitols other than inositols

Names for derivatives of cyclitols other than inositols are all constructed by applying the principles, rules, and conventions of substitutive nomenclature described in Chapters P-1 through P-9.

Examples:



(1*R*,2*S*,3*R*,4*S*,5*S*)-2,3,4,5-tetrahydroxycyclopentane-1-carboxylic acid



(1*R*,2*S*,3*R*,4*S*,5*r*)-5-aminocyclopentane-1,2,3,4-tetrol

P-105 NUCLEOSIDES

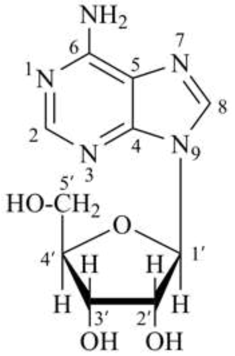
P-105.0 Introduction
P-105.1 Retained names of nucleosides
P-105.2 Substitution on nucleosides

P-105.0 INTRODUCTION

The nomenclature of nucleosides is exemplified in the document entitled ‘Abbreviations and Symbols for Nucleic Acids, Polynucleotides and their Constituents’ (ref. 47). The procedures for naming derivatives given in this Section are adapted from Section P-102 for modifications on the carbohydrate moiety and from the general rules of substitution of organic compounds.

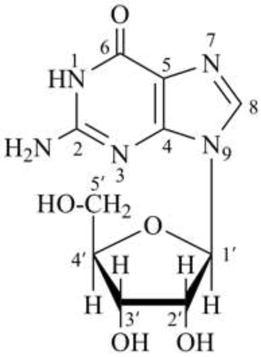
P-105.1 RETAINED NAMES OF NUCLEOSIDES

The following names are retained.



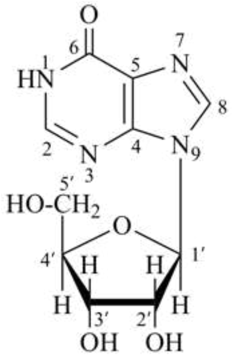
NH_2
6
7
1
N
5
N
8
2
N
4
N_9
3
5′
HO-CH_2
O
4′
H
H
1′
H
H
3′
2′
OH
OH

adenosine



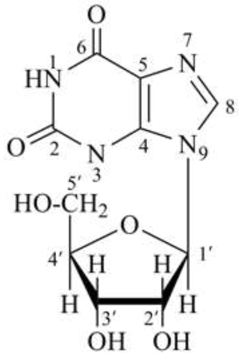
O
6
1
7
HN
5
N
8
H_2N
2
N
4
N_9
3
5′
HO-CH_2
O
4′
H
H
1′
H
H
3′
2′
OH
OH

guanosine



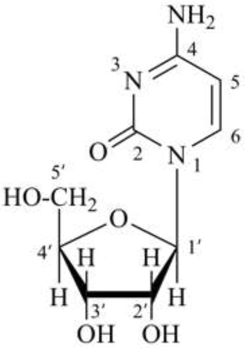
O
6
1
7
HN
5
N
8
2
N
4
N_9
3
5′
HO-CH_2
O
4′
H
H
1′
H
H
3′
2′
OH
OH

inosine



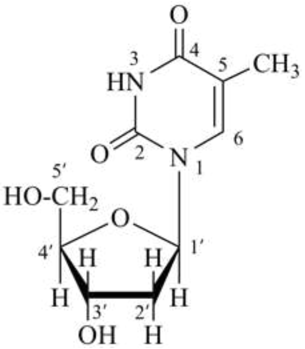
O
6
1
7
HN
5
N
8
O
2
N
4
N_9
3
5′
HO-CH_2
O
4′
H
H
1′
H
H
3′
2′
OH
OH

xanthosine

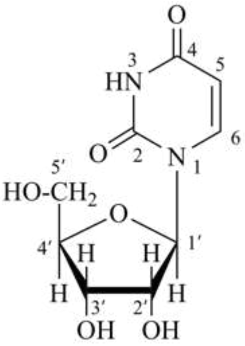


NH_2
4
3
N
5
O
2
N
1
6
5′
HO-CH_2
O
4′
H
H
1′
H
H
3′
2′
OH
OH

cytidine



thymidine

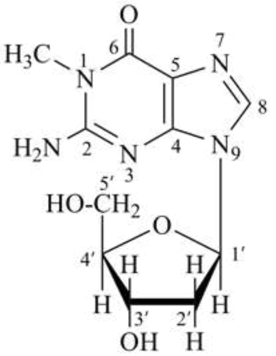


uridine

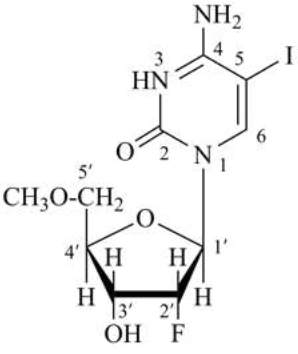
P-105.2 SUBSTITUTION ON NUCLEOSIDES

P-105.2.1 Nucleosides having retained names can be fully substituted on the purine or pyrimidine ring. Replacement of oxo groups of nucleosides is described by functional replacement prefixes. The ribofuranosyl component may be modified as prescribed for carbohydrates (see P-102.5).

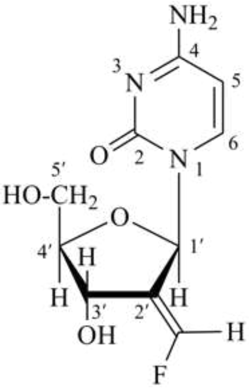
Examples:



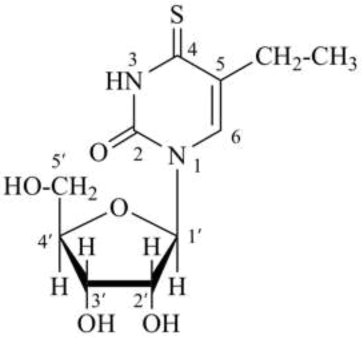
2′-deoxy-1-methylguanosine



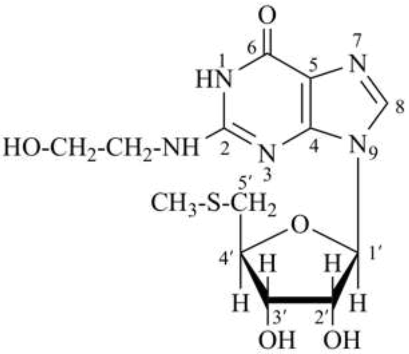
2′-deoxy-2′-fluoro-5-iodo-5′-*O*-methylcytidine
(the replacement of a hydroxy group by a fluorine atom at the same position is allowed)
4-amino-1-[(2*R*,3*R*,4*R*,5*R*)-3-fluoro-4-hydroxy-5-(methoxymethyl)oxolan-2-yl]-5-iodopyrimidin-2(1*H*)-one



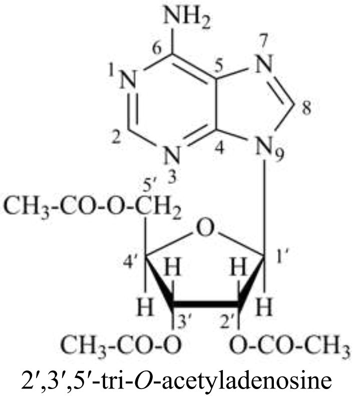
(2′*E*)-2′-deoxy-2′-(fluoromethylidene)cytidine
4-amino-1-[(2*R*,3*E*,4*S*,5*R*)-3-(fluoromethylidene)-4-hydroxy-5-(hydroxymethyl)oxolan-2-yl]pyrimidin-2(1*H*)-one



5-ethyl-4-thiouridine



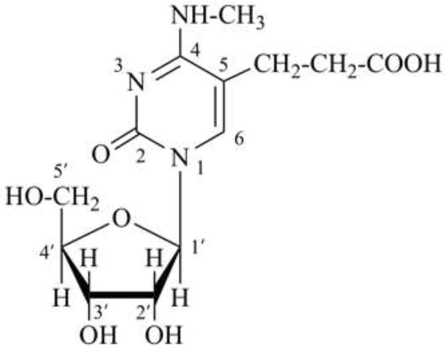
N^2-(2-hydroxyethyl)-5′-*S*-methyl-5′-thioguanosine



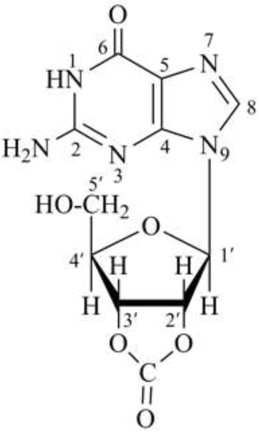
2′,3′,5′-tri-*O*-acetyladenosine
adenosine 2′,3′,5′-triacetate

P-105.2.2 In the presence of a characteristic group of higher priority than pseudoketone, normal substitutive nomenclature principles are applied.

Examples:



3-[4-(methylamino)-2-oxo-1-β-D-ribofuranosyl-1,2-dihydropyrimidin-5-yl]propanoic acid



2′,3′-dideoxyguanosine-2′,3′-diyl carbonate (see P-101.7.4)
guanosine cyclic-2′,3′-carbonate

P-106 NUCLEOTIDES

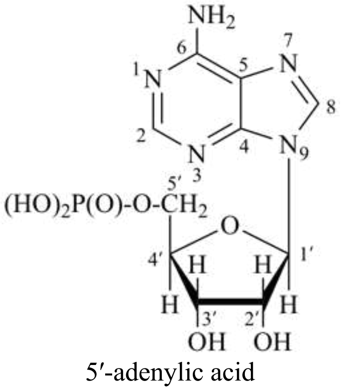
P-106.0 Introduction
P-106.1 Retained names
P-106.2 Nucleoside diphosphates and triphosphates
P-106.3 Derivatives of nucleotides

P-106.0 INTRODUCTION

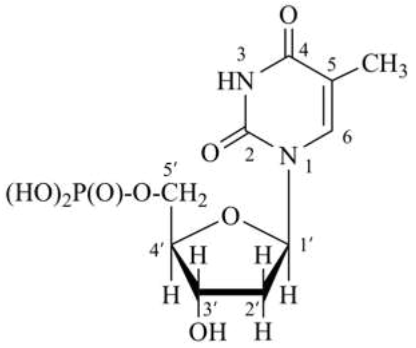
Names of nucleotides are exemplified in the document entitled ‘Abbreviations and Symbols for Nucleic Acids, Polynucleotides and their Constituents’ (ref. 47). The procedures for naming of derivatives given in this section are adapted from Section P-102 for modifications on the carbohydrate moiety and from the general rules for substitution of organic compounds.

P-106.1 RETAINED NAMES

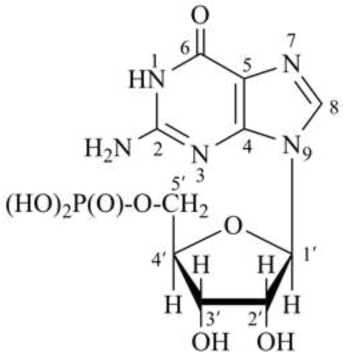
The following are traditional names for esters of nucleosides with phosphoric acid. The primed locant of the ribosyl component is cited to locate the position of the phosphate group.



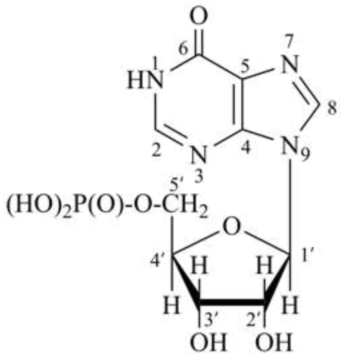
5′-adenylic acid



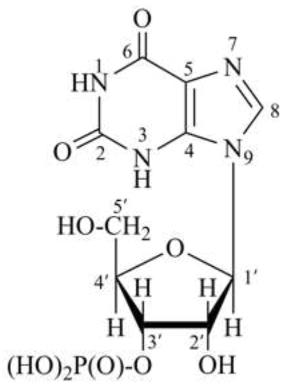
5′-thymidylic acid



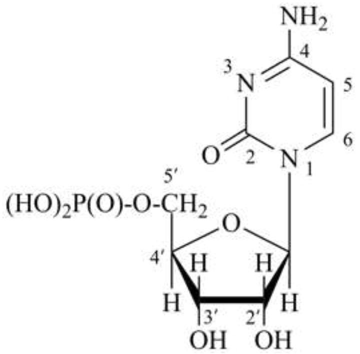
5′-guanylic acid



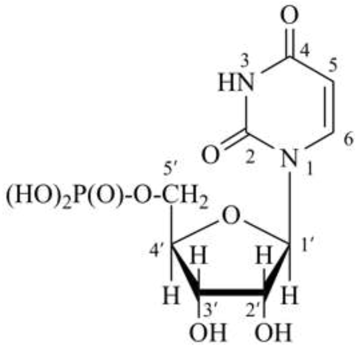
5′-inosinic acid



3′-xanthylic acid



5′-cytidylic acid

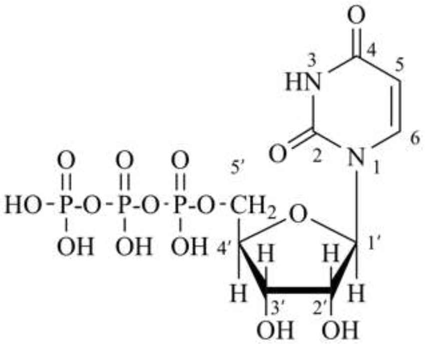


5′-uridylic acid

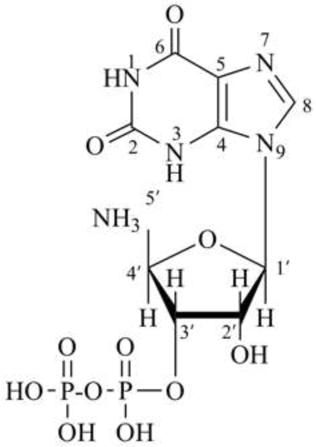
P-106.2 NUCLEOSIDE DIPHOSPHATES AND TRIPHOSPHATES

Diphosphate, triphosphate, etc. esters of nucleosides are named by citing a phrase such as diphosphate, after the name of the nucleoside. The presence of hydrogen atoms on the diphosphate, triphosphate, etc. component of the molecule is indicated by the words 'hydrogen', 'dihydrogen, etc. Parentheses are used to avoid ambiguity.

Examples:



uridine 5′-(tetrahydrogen triphosphate)

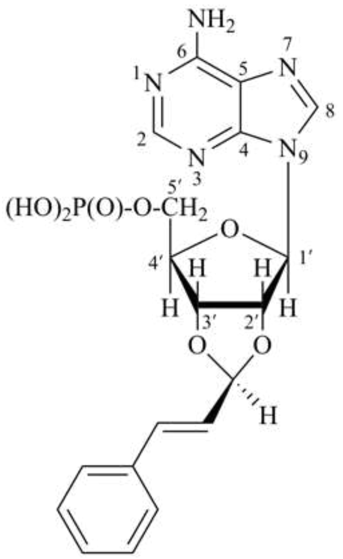


xanthosine 3′-(trihydrogen diphosphate)

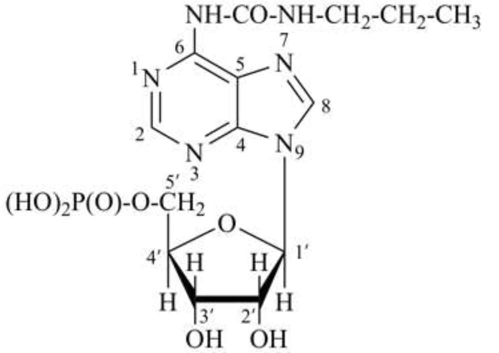
P-106.3 DERIVATIVES OF NUCLEOTIDES

P-106.3.1 Derivatives of nucleotides having retained names are named in the same manner as the corresponding nucleoside, i.e., they can be fully substituted on the purine or pyrimidine ring and the ribofuranosyl component may be modified as prescribed for carbohydrates (see P-102.5). The 2- and 3-deoxy modifications of the ribose component are also used.

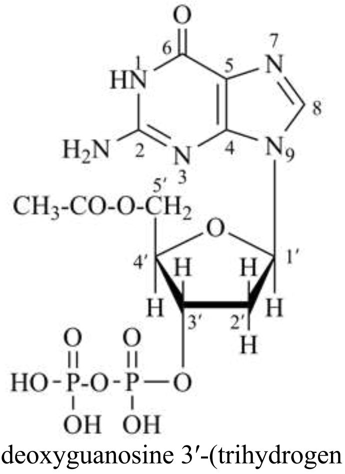
Examples:



2′,3′-*O*-[(1*S*,2*E*)-3-phenylprop-2-ene-1,1-diyl]-5′-adenylic acid



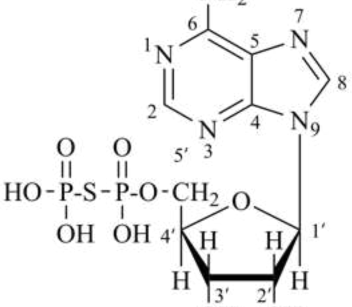
*N*⁶-(propylcarbamoyl)-5′-adenylic acid



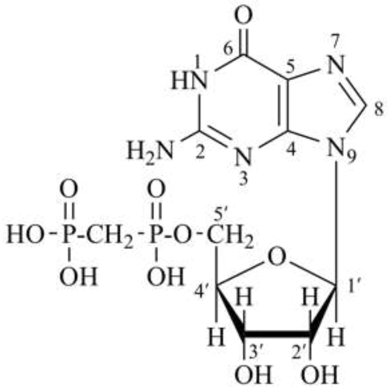
5′-*O*-acetyl-2′-deoxyguanosine 3′-(trihydrogen diphosphate)
2′-deoxyguanosine 5′-acetate 3′-(trihydrogen diphosphate)

P-106.3.2 Analogues of nucleoside di- and polyphosphates can be named by the functional replacement techniques applicable to di- and polyphosphoric acids (see P-67.2).

Examples:



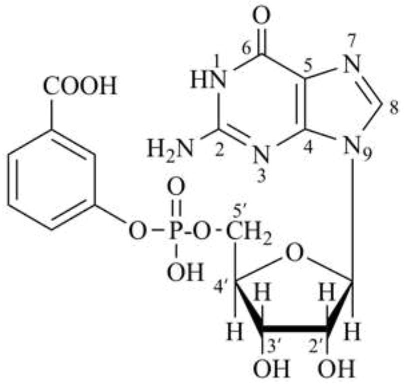
adenosine 5′-(trihydrogen 2-thiodiphosphate)



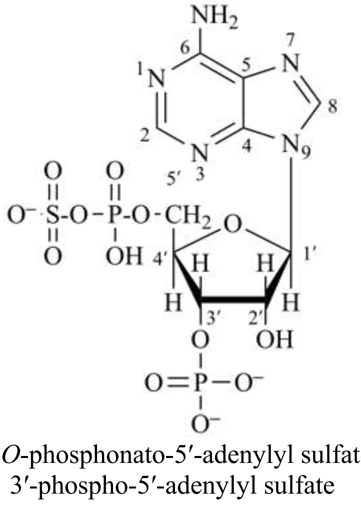
guanosine 5′-[hydrogen (phosphonomethyl)phosphonate]
guanosine 5′-(trihydrogen methylenediphosphonate)
guanosine 5′-(trihydrogen 2-carbadiphosphate)
(this name preserves the integrity of the nucleotide name; see P-101.4.3)

P-106.3.3 In the presence of a characteristic group of higher priority than the phosphoric acid residue, normal substitutive nomenclature principles are applied. Substitutive prefix names are derived from the traditional names for the nucleoside monophosphates by replacing the 'ic acid' ending with 'yl', for example, adenylyl and cytidylyl. Note that the substituent prefix name from inosinic acid is an exception; it is named inosinylyl so that the ending is like the other substituent prefix names derived from the nucleotide monophosphates.

Examples:



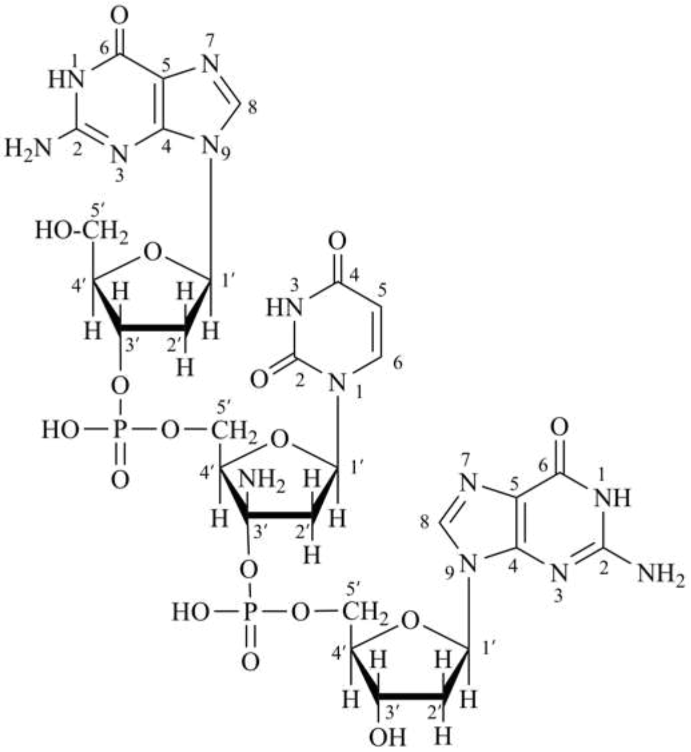
3-(5′-guanylyloxy)benzoic acid



3′-*O*-phosphonato-5′-adenylyl sulfate
3′-phospho-5′-adenylyl sulfate

P-106.3.4 Oligonucleotides are named using the prefix names derived from the traditional names for the nucleotides.

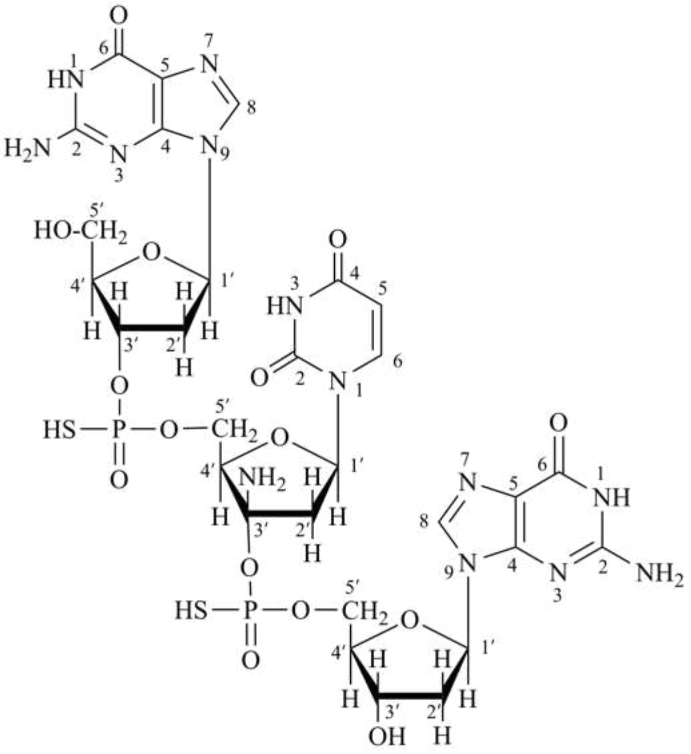
Example:



2′-deoxyguanylyl-(3′→5′)-2′-deoxyuridylyl-(3′→5′)-2′-deoxyguanosine

P-106.3.5 When a phosphorothioic acid is used (HS-P in place of HO-P), the prefix *P*-thio is added at the front of the name of the nucleotide.

Example:



2′-deoxy-*P*-thioguanylyl-(3′→5′)-2′-deoxy-*P*-thiouridylyl-(3′→5′)-2′-deoxyguanosine

P-107 LIPIDS

P-107.0 Introduction
P-107.1 Definitions
P-107.2 Glycerides
P-107.3 Phosphatidic acids
P-107.4 Glycolipids

P-107.0 INTRODUCTION

The nomenclature of lipids, phospholipids, and glycolipids has been published in 1976 (ref. 48); the nomenclature of glycolipids was revised in 1997 (ref. 50).

P-107.1 DEFINITIONS

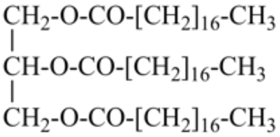
'Lipids' is a loosely defined term for substances of biological origin that are soluble in nonpolar solvents. They consist of saponifiable lipids, such as 'glycerides' (fats and oils) and 'phospholipids', as well as nonsaponifiable lipids, specifically 'steroids'.

The nomenclature of lipids, like that of carbohydrates, is composed of retained names and systematic names constructed in the context of the specialized lipid nomenclature. The name 'sphinganine' for '(2*S*,3*R*)-2-aminoctadecane-1,3-diol' is retained in lipid nomenclature for the diol itself and its derivatives.

P-107.2 GLYCERIDES

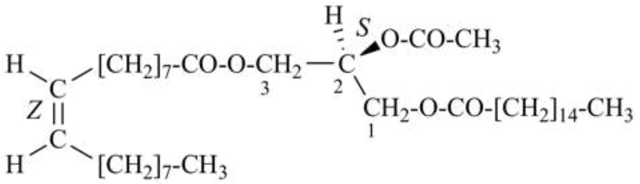
Glycerides are esters of glycerol (propane-1,2,3-triol) with fatty acids. They are by long established custom subdivided into triglycerides, 1,2- or 1,3-diglycerides, and 1- or 2-monoglycerides, according to the number and position of the acyl groups. Individual glycerides are named as mono-, di- or tri-*O*-acylglycerol. The name glycerol is allowed in general nomenclature to name organic compounds; it is also a retained name in the field of natural products, especially in the nomenclature of lipids.

Examples:



$$\begin{array}{l}\mathrm{CH_2\text{-}O\text{-}CO\text{-}[CH_2]_{16}\text{-}CH_3}\\ |\\ \mathrm{CH\text{-}O\text{-}CO\text{-}[CH_2]_{16}\text{-}CH_3}\\ |\\ \mathrm{CH_2\text{-}O\text{-}CO\text{-}[CH_2]_{16}\text{-}CH_3}\end{array}$$

tri-*O*-octadecanoylglycerol
propane-1,2,3-triyl trioctadecanoate



(2*S*)-2-*O*-acetyl-1-*O*-hexadecanoyl-3-*O*-[(9*Z*)-octadec-9-enoyl]glycerol (numbering shown)
(2*S*)-2-*O*-acetyl-1-*O*-oleoyl-3-*O*-palmitoylglycerol
(2*S*)-propane-1,2,3-triyl 2-acetate 1-hexadecanoate 3-[(9*Z*)-octadec-9-enoate]

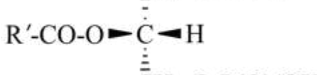
Phospholipids are lipids containing phosphoric acid as mono- or diesters, including 'phosphatidic acids' and 'phosphoglycerides'.

Phosphatidic acids are derivatives of glycerol in which one hydroxy group, commonly but not necessarily primary, is esterified with phosphoric acid, and the other two hydroxy groups are esterified with fatty acids.

Phosphoglycerides are phosphoric diesters, esters of phosphatidic acids, generally having a polar head group (–OH or $-NH_2$) on the esterified alcohol which typically is 2-aminoethanol (not 'ethanolamine'), choline, glycerol, inositol, or serine. The term includes 'lecithins' and 'cephalins'.

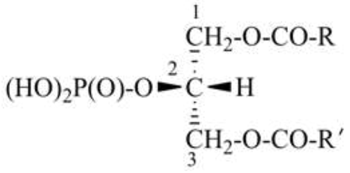
P-107.3 PHOSPHATIDIC ACIDS

P-107.3.1 Phosphatidic acids have the following generic structure:



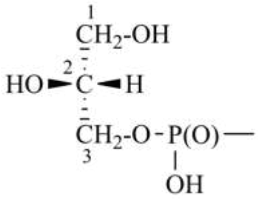
a 3-*sn*-phosphatidic acid
(for a discussion and examples of '*sn*' see P-107.3.2)

In general, the 3-*sn*-phosphatidic acids are simply called phosphatidic acids.



a 2-phosphatidic acid

The name of the monovalent acyl group is 'phosphatidyl', a retained name.



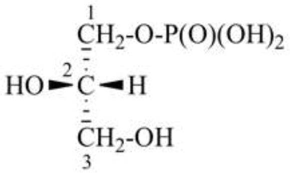
phosphatidyl

P-107.3.2 Configuration of phosphatidic acids

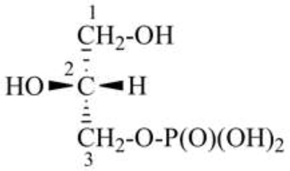
In order to designate the configuration of glycerol derivatives, the carbon atoms of glycerol are numbered by a method referred to as 'stereospecific numbering'. The carbon atom that appears on top of that Fischer projection that shows a vertical carbon chain with the hydroxy group at carbon 2 to the left is designated as C-1.

To differentiate such numbering from conventional numbering, which conveys no steric information, the stereodescriptor '*sn*' (for 'stereospecifically numbered') is used. This descriptor is written in lower-case italics, even at the beginning of a sentence, immediately preceding the glycerol term, from which it is separated by a hyphen. The stereodescriptor '*rac*' is used to describe racemates and the stereodescriptor '*Ξ*' may be used if the configuration of the compound is unknown or unspecified.

Examples:



sn-glycerol 1-phosphate
(2*S*)-2,3-dihydroxypropyl dihydrogen phosphate

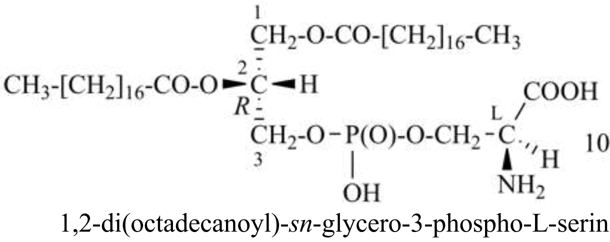


sn-glycerol 3-phosphate
(2*R*)-2,3-dihydroxypropyl dihydrogen phosphate

P-107.3.3 Phosphatidylserines

The term 'phosphatidylserines' is used to describe the acyl derivatives of phosphatidic acids whose phosphorus acid component is esterified with the amino acid 'serine', usually L-serine. Semisystematic names of specific compounds are formed in accordance with the principles, rules, and conventions of substitutive nomenclature.

Example:



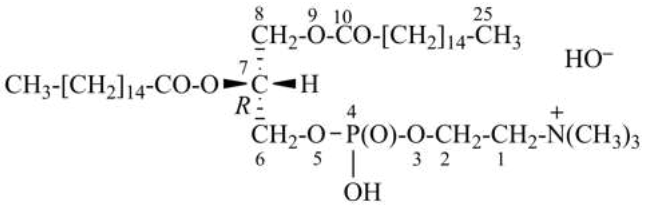
107330a

1,2-di(octadecanoyl)-*sn*-glycero-3-phospho-L-serine
O-{[(2*R*)-2,3-bis(octadecanoyloxy)propoxy]hydroxyphosphoryl}-L-serine

P-107.3.4 Phosphatidylcholines

The term 'phosphatidylcholines' is used to describe the acyl derivatives of phosphatidic acids whose phosphorus acid component is esterified with choline. Semisystematic names of specific compounds are formed in accordance with the principles, rules, and conventions of substitutive nomenclature.

Example:

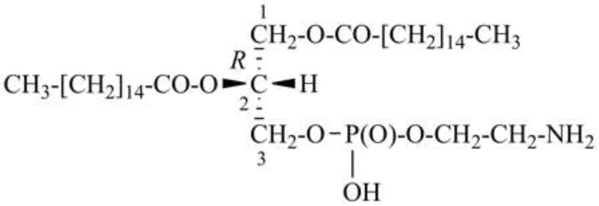


(7*R*)-7-(hexadecanoyloxy)-4-hydroxy-*N*,*N*,*N*-trimethyl-4,10-dioxo-3,5,9-trioxa-$4\lambda^5$-phosphapentacosan-1-aminium hydroxide

P-107.3.5 Phosphatidylethanolamine

The term ‘phosphatidylethanolamines’ [more correctly designated as ‘phosphatidyl(amino)ethanols’] is used to describe the acyl derivatives of phosphatidic acids whose phosphorus acid component is esterified with 2-aminoethanol. Semisystematic names for specific compounds are formed in accordance with the principles, rules, and conventions of substitutive nomenclature.

Example:

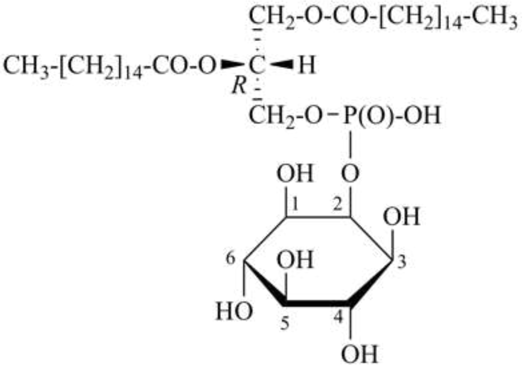


1,2-di(hexadecanoyl)-*sn*-glycero-3-phosphoethanolamine
(2*R*)-3-{[(2-aminoethoxy)hydroxyphosphoryl]oxy}propane-1,2-diyl di(hexadecanoate)

P-107.3.6 Phosphatidylinositols

The term ‘phosphatidylinositols’ is used to describe the acyl derivatives of phosphatidic acids whose phosphorus acid component is esterified with an inositol molecule. Semisystematic names for specific compounds are formed in accordance with the principles, rules, and conventions of substitutive nomenclature.

Example:



L-*myo*-inositol 2-[(2*R*)-2,3-bis(hexadecanoyloxy)propyl hydrogen phosphate]
(2*R*)-3-[(hydroxy{[(1*s*,2*R*,3*R*,4*s*,5*S*,6*S*)-2,3,4,5,6-pentahydroxycyclohexyl]oxy}phosphoryl)oxy]propane-1,2-diyl di(hexadecanoate)

P-107.4 GLYCOLIPIDS

P-107.4.1 Definitions

The term ‘glycolipid’ designates any compound containing one or more monosaccharide residues bound by a glycosidic linkage to a hydrophobic moiety such as an acyl glycerol, a sphingoid (a long chain aliphatic amino alcohol), a ceramide (an *N*-acyl-sphingoid), or a prenylphosphate.

Glycoglycerolipids are glycolipids containing one or more glycerol residues.

Glycosphingolipids designate lipids containing at least one monosaccharide residue and either a sphingoid or a ceramide.

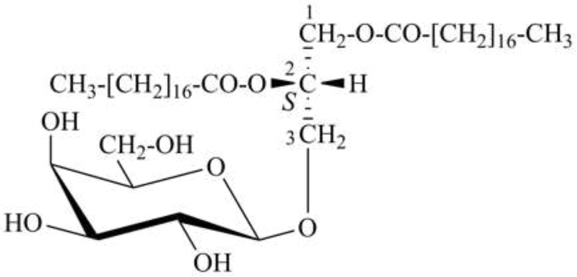
The term ‘glycophosphatidylinositol’ designates glycolipids which contain saccharides glycosidically linked to the inositol moiety of phosphatidylinositols.

Specific compounds are named systematically.

P-107.4.2 Glycoglycerolipids

Specific compounds are named on the basis of the parent glycerol, whose configuration is specifically numbered as indicated in P-107.3.2]

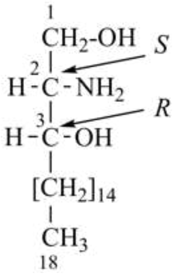
Example:



3-*O*-β-D-galactopyranosyl-1,2-di-*O*-octadecanoyl-*sn*-glycerol
(2*S*)-3-(β-D-galactopyranosyloxy)propane-1,2-diyl dioctadecanoate

P-107.4.3 Glycosphingolipids

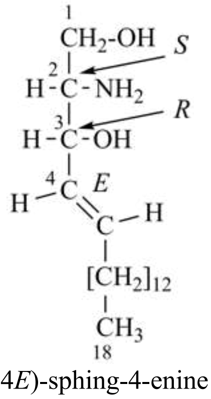
P-107.4.3.1 Names are formed by using the retained name ‘sphinganine’ for the aliphatic amino alcohol having the described absolute configuration. The retained name ‘sphinganine’ is preferred to the systematic name (2*S*,3*R*)-2-aminooctadecane-1,3-diol.



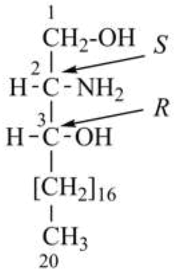
sphinganine
(2*S*,3*R*)-2-aminooctadecane-1,3-diol

The retained name sphinganine is used to generate the names of unsaturated and *N*-substituted derivatives, as well as *O*-substituted derivatives. Other derivatives, such as hydroxy, oxo, and amino derivatives, as well as isomers with different chain length or other diastereoisomers, are named systematically in accordance with the principles, rules, and conventions of substitutive nomenclature.

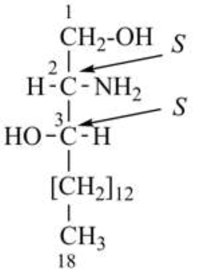
Examples:



(4*E*)-sphing-4-enine
(2*S*,3*R*,4*E*)-2-aminooctadec-4-ene-1,3-diol



icosasphinganine
(2*S*,3*R*)-2-aminoicosane-1,3-diol

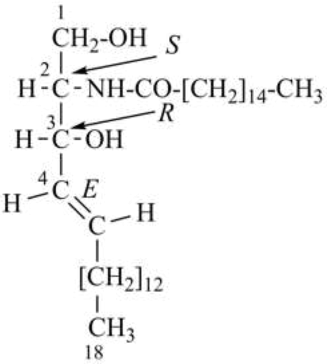


(2*S*,3*S*)-2-aminooctadecane-1,3-diol

P-107.4.3.2 Ceramides

Ceramides are *N*-acylsphingoids.

Example:

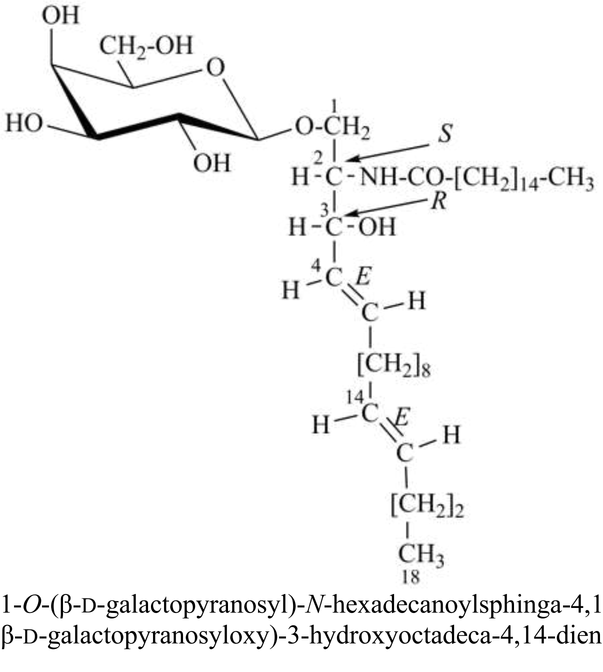


(4*E*)-*N*-hexadecanoylsphing-4-enine
N-[(2*S*,3*R*,4*E*)-1,3-dihydroxyoctadec-4-en-2-yl]hexadecanamide

P-107.4.3.3 Neutral glycosphingolipids

A neutral glycosphingolipid is a carbohydrate-containing derivative of a sphingoid or ceramide. It is understood that the carbohydrate residue is attached by a glycosidic linkage to 1-*O*-. Preferred systematic names must include all locants.

Example:



(4*E*,14*E*)-1-*O*-(β-D-galactopyranosyl)-*N*-hexadecanoylsphinga-4,14-dienine
N-[(2*S*,3*R*,4*E*,14*E*)-1-(β-D-galactopyranosyloxy)-3-hydroxyoctadeca-4,14-dien-2-yl]hexadecanamide

International Union of Pure and Applied Chemistry

Division VIII Chemical Nomenclature and Structure Representation Division

Nomenclature of Organic Chemistry. IUPAC Recommendations and Preferred Names 2013.

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Appendix 1

Seniority list of elements and ‘a’ terms used in skeletal replacement (‘a’) nomenclature, in decreasing order of seniority

Element	‘a’ Term
F	fluora
Cl	chlora
Br	broma
I	ioda
At	astata
O	oxa
S	thia
Se	selena
Te	tellura
Po	polona
Lv	livermora
N	aza
P	phospha
As	arsa
Sb	stiba
Bi	bisma
C	carba
Si	sila
Ge	germa
Sn	stanna
Pb	plumba
Fl	flerova
B	bora
Al	alumina
Ga	galla
In	inda
Tl	thalla
Zn	zinca
Cd	cadma
Hg	mercura
Cn	copernica
Cu	cupra
Ag	argenta
Au	aura
Rg	roentgena
Ni	nickela

Pd	pallada
Pt	platina
Ds	darmstadta
Co	cobalta
Rh	rhoda
Ir	irida
Mt	meitnera
Fe	ferra
Ru	ruthena
Os	osma
Hs	hassa
Mn	mangana
Te	techneta
Re	rhena
Bh	bohra
Cr	chroma
Mo	molybda
W	tungsta
Sg	seaborga
V	vanada
Nb	nioba
Ta	tantala
Db	dubna
Ti	titana
Zr	zircona
Hf	hafna
Rf	rutherforda
Sc	scanda
Y	yttra
La	lanthana
Ce	cera
Pr	praseodyma
Nd	neodyma
Pm	prometha
Sm	samara
Eu	europa
Gd	gadolina
Tb	terba
Dy	dysprosa
Ho	holma
Er	erba
Tm	thula
Yb	ytterba
Lu	luteta
Ac	actina
Th	thora
Pa	protactina
U	urana

Np	neptuna
Pu	plutona
Am	america
Cm	cura
Bk	berkela
Cf	californa
Es	einsteina
Fm	ferma
Md	mendeleva
No	nobela
Lr	lawrenca
Be	berylla
Mg	magnesa
Ca	calca
Sr	stronta
Ba	bara
Ra	rada
Li	litha
Na	soda
K	potassa
Rb	rubida
Cs	caesa
Fr	franca
He	hela
Ne	neona
Ar	argona
Kr	kryptona
Xe	xenona
Rn	radona

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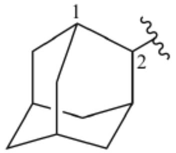
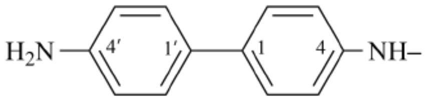
Appendix 2

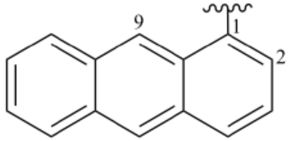
DETACHABLE PREFIXES USED FOR SUBSTITUTIVE NOMENCLATURE

The symbol * designates the preferred prefix (for example: acetamido* = acetylamino; acetylamino = acetamido*) or the preselected prefix (for example: sulfanyl* = thio).

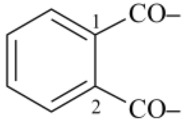
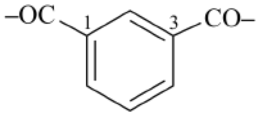
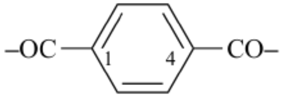
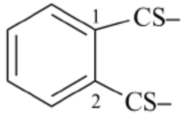
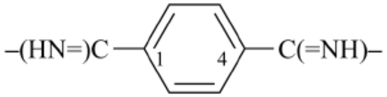
Prefixes that are not recommended are followed by the mention 'see' followed by the preferred or preselected prefix (for example: 'chloroxy: see chloryl*'. No formula is given for the entry 'chloroxy'. As a counterpart, the preferred or preselected prefix is followed by the mention 'not' and the prefix that is not recommended enclosed in appropriate enclosing marks [for example: chloryl* (not chloroxy)].

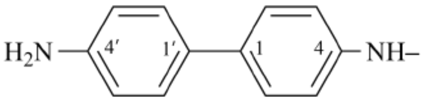
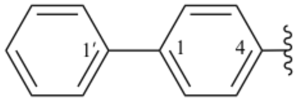
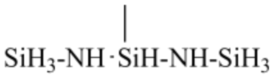
Name	Formula	Rule(s)
acetamido* = acetylamino	CH_3-CO-NH–	P-66.1.1.4.3
acetimidamido = ethanimidamido* = acetimidoylamino	CH_3-C(=NH)-NH–	P-66.4.1.3.5
acetimidoyl = ethanimidoyl* = 1-iminoethyl	CH_3-C(=NH)–	P-65.1.7.2.2
acetimidoylamino = ethanimidamido* = acetimidamido	CH_3-C(=NH)-NH–	P-66.4.1.3.5
acetohydrazido* = 2-acetylhydrazin-1-yl	CH_3-CO-NH-NH–	P-66.3.2.3
acetohydrazonoyl = ethanehydrazonoyl* = 1-hydrazinylideneethyl	CH_3-C(=N-NH_2)–	P-65.1.7.2.2
acetohydroximoyl = *N*-hydroxyethanimidoyl* = *N*-hydroxyacetimidoyl	CH_3C(=N-OH)–	P-65.1.7.2.2
acetonyl = 2-oxopropyl*	$\overset{3}{\mathrm{C}}\mathrm{H_3}\text{-}\overset{2}{\mathrm{C}}\mathrm{O}\text{-}\overset{1}{\mathrm{C}}\mathrm{H_2}\text{–}$	P-64.5.1
acetonylidene: see 2-oxopropylidene*		
acetonylidyne: see 2-oxopropylidyne*		
acetoxy = acetyloxy*	CH_3-CO-O–	P-65.6.3.2.3
acetoxysulfonyl = (acetyloxy)sulfonyl*	CH_3-CO-O-SO_2–	P-65.3.2.3
acetyl* = ethanoyl = 1-oxoethyl	CH_3-CO–	P-65.1.7.2.1
N-acetylacetamido* = diacetylamino (not diacetylazanyl; not diacetamido)	$(CH_3\text{-}CO)_2N$–	P-66.1.2.1
acetylamino = acetamido*	CH_3-CO-NH–	P-66.1.1.4.3
acetylazanediyl* (not acetylimino)	CH_3-CO-N<	P-66.1.1.4.4
acetylazanylidene* = acetylimino	CH_3-CO-N=	P-62.3.1.2

2-acetylhydrazin-1-yl = acetohydrazido*	CH_3-CO-NH-NH–	P-66.3.2.3
acetylimino = acetylazanylidene* (not acetylazanediyl)	CH_3-CO-N=	P-62.3.1.2
acetyloxy* = acetoxy	CH_3-CO-O–	P-65.6.3.2.3
(acetyloxy)sulfonyl* = acetoxysulfonyl	CH_3-CO-O-SO_2–	P-65.3.2.3
acrylohydrazonoyl = prop-2-enehydrazonoyl* = 1-hydrazinylideneprop-2-en-1-yl	CH_2=CH-C(=N-NH_2)–	P-65.1.7.3.2
acryloyl = prop-2-enoyl* = 1-oxoprop-2-en-1-yl	CH_2=CH-CO–	P-65.1.7.3.1; P-65.1.7.4.1
adamantan-2-yl* = 2-adamantyl = tricyclo[3.3.1.1^{3,7}]decan-2-yl (also 1-isomer) 2-adamantyl = adamantan-2-yl* = tricyclo[3.3.1.1^{3,7}]decan-2-yl (also 1-isomer)		P-29.6.2.3; P-57.1.5.3
adipoyl = hexanedioyl* = 1,6-dioxohexane-1,6-diyl	–CO-[CH_2]$_4$-CO–	P-65.1.7.3.1; P-65.1.7.4.1
allyl = prop-2-en-1-yl*	CH_2=CH-CH_2–	P-32.3
allylidene = prop-2-en-1-ylidene*	CH_2=CH-CH=	P-32.3
allylidyne = prop-2-enylidyne*	CH_2=CH-C≡	P-32.3
alumanyl*	H_2Al–	P-29.3.1; P-68.1.2
alumanylidene*	HAl=	P-29.3.1; P-68.1.2
amidino: see carbamimidoyl*		
amidochlorophosphoryl = phosphoramidochloridoyl* (not chloroamidophosphoryl)	(H_2N)ClP(O)–	P-67.1.4.1.1.4
amidyl = azanidyl*	$^{-}$NH–	P-72.6.3
amidylidene = azanidylidene*	$^{-}$N=	P-72.6.3
amino* = azanyl	H_2N–	P-62.2.3
(4′-amino[1,1′-biphenyl]-4-yl)amino* = benzidino		P-62.2.4.1.1
C-aminocarbonimidoyl = carbamimidoyl* = amino(imino)methyl (not amidino)	H_2N-C(=NH)–	P-65.2.1.5; P-66.4.1.3.1
aminocarbonothioyl = carbamothioyl* = amino(sulfanylidene)methyl (not thiocarbamoyl)	H_2N-CS–	P-65.2.1.5; P-66.1.4.4
aminocarbonyl = carbamoyl*	H_2N-CO–	P-65.2.1.5; P-66.1.1.4.1.1
(aminocarbonyl)amino = carbamoylamino* (not ureido)	H_2N-CO-NH–	P-66.1.6.1.1.3
[(aminocarbonyl)amino]carbonyl = carbamoylcarbamoyl*	H_2N-CO-NH-CO–	P-66.1.6.1.1.4
2-(aminocarbonyl)hydrazin-1-yl = 2-carbamoylhydrazin-1-yl* = semicarbazido	H_2N-CO-NH-NH–	P-68.3.1.2.4
aminodichlorosilyl*	(H_2N)Cl_2Si–	P-67.1.4.2
amino(hydrazinylidene)methyl = carbamohydrazonoyl*	H_2N-C(=N-NH_2)–	P-66.4.2.3.2
[amino(hydroxy)methylidene]amino* (not 3-isoureido)	H_2N-C(OH)=N–	P-66.1.6.1.2.2
amino(imino)methyl = carbamimidoyl* = *C*-aminocarbonimidoyl (not amidino)	H_2N-C(=NH)–	P-65.2.1.5; P-66.4.1.3.1
[amino(imino)methyl]amino = carbamimidoylamino* = carbamimidamido = guanidino	H_2N-C(=NH)-NH–	P-66.4.1.2.1.3
(aminomethylidene)amino*	H_2N-CH=N–	P-66.4.1.3.3

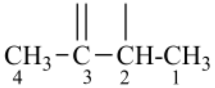
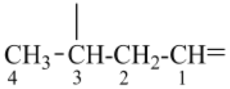
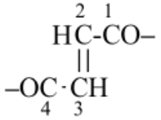
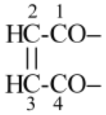
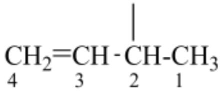
(aminomethylidene)hydrazinyl*	H_2N-CH=N-NH–	P-66.4.2.3.4
aminooxalyl = oxamoyl* = amino(oxo)acetyl (not carbamoylformyl; not carbamoycarbonyl)	H_2N-CO-CO–	P-66.1.1.4.1.2
amino(oxo)acetamido = oxamoylamino* (not carbamoylformamido)	H_2N-CO-CO-NH–	P-66.1.1.4.5.1
amino(oxo)acetyl = oxamoyl* = aminooxalyl (not carbamoylformyl; not carbamoycarbonyl)	H_2N-CO-CO–	P-66.1.1.4.1.2
[amino(oxo)acetyl]imino = oxamoylimino*	H_2N-CO-CO-N=	P-66.1.1.4.5.1
aminooxy* (not aminoxy)	H_2N-O–	P-68.3.1.1.1.5
amino(sulfanylidene)methyl = carbamothioyl* = aminocarbonothioyl (not thiocarbamoyl)	H_2N-CS–	P-65.2.1.5; P-66.1.4.4
[amino(sulfanylidene)methyl]amino = carbamothioylamino*	H_2N-CS-NH–	P-66.1.6.1.3.3
[amino(sulfanyl)methylidene]amino*	H_2N-C(SH)=N–	P-66.1.6.1.3.3
S-aminosulfinimidoyl*	H_2N-S(=NH)–	P-66.4.1.3.4
aminosulfinyl* (not sulfinamoyl)	H_2N-S(O)–	P-66.1.1.4.2
(aminosulfinyl)oxy* (not sulfinamoyloxy)	H_2N-S(O)-O–	P-67.1.4.4.2
S-aminosulfonimidoyl*	H_2N-S(O)(=NH)–	P-66.4.1.3.4
S-aminosulfonodiimidoyl*	H_2N-S(=NH)$_2$–	P-66.4.1.3.4
aminosulfonyl = sulfamoyl* = sulfuramidoyl	H_2N-SO_2–	P-65.3.2.3; P-66.1.1.4.2
aminoxy: see aminooxy*		
ammonio = azaniumyl* = ammoniumyl	H_3N^+–	P-73.6
ammoniumyl = azaniumyl* = ammonio	H_3N^+–	P-73.6
anilino* = phenylamino	C_6H_5-NH–	P-62.2.1.1.1
anilinosulfonyl = phenylsulfamoyl* = (phenylamino)sulfonyl	C_6H_5-NH-SO_2–	P-66.1.1.4.2
o-anisidino: see 2-methoxyanilino* (also *m* = 3- and *p* = 4-isomers)		
2-anisidino: see 2-methoxyanilino*		
anthracen-1-yl* = 1-anthryl (also 2-, 9-isomers) 1-anthryl = anthracen-1-yl* (also 2-, 9-isomers)		P-29.6.2.3; P-57.1.5.3
antimonyl: see stiboryl*		
arsanediyl* (not arsinediyl)	HAs<	P-68.3.2.3.2.2
arsanetriyl* (not arsinetriyl)	–As<	P-68.3.2.3.2.2
arsaniumyl* = arsonio = arsoniumyl	H_3As^+–	P-73.6
arsanyl* = arsino	H_2As–	P-29.3.1; P-68.3.2.3.2.2
λ^5-arsanyl* = arsoranyl	H_4As–	P-68.3.2.3.2.2
arsanylidene* (not arsinidine)	HAs=	P-29.3.1; P-68.3.2.3.2.2
arsenoso: see oxoarsanyl*		
arsenyl: see arsoryl*		
arsinediyl: see arsanediyl*		

arsinetriyl: see arsanetriyl*		
arsinidine: see arsanylidene*		
arsino = arsanyl*	H_2As–	P-29.3.1; P-68.3.2.3.2.2
arsinoyl* = dihydroarsoryl (not arsinyl)	$H_2As(O)$–	P-67.1.4.1.1.2; P-67.1.4.1.2
arsinyl: see arsinoyl*		
arso: see dioxo-λ^5-arsanyl*		
arsonato*	$(^{-}O)_2As(O)$–	P-72.6.1
arsonio = arsaniumyl* = arsoniumyl	H_3As^{+}–	P-73.6
arsoniumyl = arsaniumyl* = arsonio	H_3As^{+}–	P-73.6
arsono* = dihydroxyarsoryl	$(HO)_2As(O)$–	P-67.1.4.1.1.1
arsonoyl* = hydroarsoryl	HAs(O)<	P-67.1.4.1.1.2; P-67.1.4.1.2
arsoranyl = λ^5-arsanyl*	H_4As–	P-68.3.2.3.2.2
arsorimidoyl* = imidoarsoryl	As(=NH)<	P-67.1.4.1.1.4
arsoryl* (not arsenyl)	–As(O)<	P-67.1.4.1.1.2
azanediidyl*	N^{2-}–	P-72.6.3
azanediyl* (not imino)	HN<	P-35.2.2; P-62.2.5.1
azanetriyl = nitrilo* (not azanylidyne; not azanylylidene)	–N<	P-35.2.1; P-62.2.5.1
azanidyl* = amidyl	^{-}NH–	P-72.6.3
azanidylidene* = amidylidene	^{-}N=	P-72.6.3
azaniumyl* = ammonio = ammoniumyl	H_3N^{+}–	P-73.6
azanyl = amino*	H_2N–	P-62.2.3
azanylidene = imino*	HN=	P-35.2.1;;P-62.3.1.2
azanylidyne* (not nitrilo)	N≡	P-35.2.2
azanylylidene* (not nitrilo)	–N=	P-35.2.2; P-62.3.1.2
azido*	N_3–	P-61.7
azino: see hydrazinediylidene*		
azinoyl* = dihydronitroryl (not azinyl)	$H_2N(O)$–	P-67.1.4.1.1.2; P-67.1.4.1.2
azinyl: see azinoyl*		
azo = diazenediyl*	–N=N–	P-32.1.1; P-68.3.1.3.2.1; P-68.3.1.3.2.2
azonato*	$(^{-}O_2$–N(O)–	P-72.6.1
azono* = dihydroxynitroryl	$(HO)_2N(O)$–	P-67.1.4.1.1.1; P-67.1.4.1.1.5
azonothioyl* = thioazonoyl	HN(S)<	P-67.1.4.1.1.4
azonoyl* = hydronitroryl	HN(O)<	P-67.1.4.1.1.2; P-67.1.4.1.2
azoryl: see nitroryl*		
NNO-azoxy	–N=N(O)–	P-68.3.1.3.3.1
NON-azoxy	–N(O)=N– or –N=N(O)–	P-68.3.1.3.3.1

ONN-azoxy	–N(O)=N–	P-68.3.1.3.3.1
benzal: see benzylidene*		
benzamido* = benzoylamino	C_6H_5-CO-NH–	P-66.1.1.4.3
benzenecarbohydroximoyl = *N*-hydroxybenzenecarboximidoyl* = *N*-hydroxybenzimidoyl = benzhydroximoyl	C_6H_5-C(=N-OH)–	P-65.1.7.2.2
benzenecarbonyl = benzoyl*= oxo(phenyl)methyl = phenylcarbonyl	C_6H_5-CO–	P-34.2.1.1; P-34.2.2; P-65.1.7.2.1
benzenecarbothioamido* = (benzenecarbothioyl)amino = thiobenzamido	C_6H_5-CS-NH–	P-66.1.4.4
benzenecarbothioyl* = thiobenzoyl = phenyl(sulfanylidene)methyl = phenyl(thioxo)methyl	C_6H_5-CS–	P-65.1.7.2.3
(benzenecarbothioyl)amino = benzenecarbothioamido* = thiobenzamido	C_6H_5-CS-NH–	P-66.1.4.4
benzenecarboximidohydrazido* = 2-(benzenecarboximidoyl)hydrazin-1-yl	C_6H_5-C(=NH)-NH-NH–	P-66.4.2.3.6
benzenecarboximidoyl* = benzimidoyl = imino(phenyl)methyl	C_6H_5-C(=NH)–	P-65.1.7.2.2
2-(benzenecarboximidoyl)hydrazin-1-yl = benzenecarboximidohydrazido*	C_6H_5-C(=NH)-NH-NH–	P-66.4.2.3.6
benzene-1,2-dicarbonyl* = phthaloyl = 1,2-phenylenedicarbonyl = 1,2-phenylenebis(oxomethylene)		P-65.1.7.3.1; P-65.1.7.4.2
benzene-1,3-dicarbonyl* = isophthaloyl = 1,3-phenylenedicarbonyl = 1,3-phenylenebis(oxomethylene)		P-65.1.7.3.1; P-65.1.7.4.2
benzene-1,4-dicarbonyl* = terephthaloyl = 1,4-phenylenedicarbonyl = 1,4-phenylenebis(oxomethylene)		P-65.1.7.3.1; P-65.1.7.4.2
benzene-1,2-dicarbothioyl* = 1,2-phenylenebis(sufanylidenemethylene) = 1,2-phenylenebis(thioxomethylene) (not dithiophthaloyl) (also 1,3- and 1,4-isomers)		P-65.1.7.3.1; P-65.1.7.4.3
benzene-1,4-dicarboximidoyl* = terephthalimidoyl = 1,4-phenylenebis(iminomethylene) = 1,4-phenylenedicarbonimidoyl (also phthalimidoyl = 1,2-isomer; and isophthalimidoyl = 1,3-isomer)		P-65.1.7.3.2
benzene-1,2-diyl: see 1,2-phenylene* (also 1,3- and 1,4-isomers)		
benzeneselenonyl* = phenylselenonyl	C_6H_5-SeO_2–	P-65.3.2.2.2
benzenesulfinamido* = (benzenesulfinyl)amino = (phenylsulfinyl)amino	C_6H_5-S(O)-NH–	P-66.1.1.4.3
benzenesulfinohydrazonamido* = (benzenesulfinohydrazonoyl)amino	C_6H_5-S(=N-NH_2)-NH–	P-66.4.2.3.5
(benzenesulfinohydrazonoyl)amino = benzenesulfinohydrazonamido*	C_6H_5-S(=N-NH_2)-NH–	P-66.4.2.3.5
benzenesulfinoselenoyl* = phenylsulfinoselenoyl	C_6H_5-S(Se)–	P-65.3.2.2.2
benzenesulfinyl* = phenylsulfinyl	C_6H_5-S(O)–	P-63.6; P-65.3.2.2.2
(benzenesulfinyl)amino = benzenesulfinamido* = (phenylsulfinyl)amino	C_6H_5-S(O)-NH–	P-66.1.1.4.3

benzenesulfonamido* = (benzenesulfonyl)amino = (phenylsulfonyl)amino	C_6H_5-SO_2-NH–	P-66.1.1.4.3
benzenesulfonyl* = phenylsulfonyl	C_6H_5-SO_2–	P-63.6; P-65.3.2.2.2
(benzenesulfonyl)amino = benzenesulfonamido* = (phenylsulfonyl)amino	C_6H_5-SO_2-NH–	P-66.1.1.4.3
benzhydryl: see diphenylmethyl*		
benzidino = (4′-amino[1,1′-biphenyl]-4-yl)amino*		P-62.2.4.1.1
benzimidoyl = benzenecarboximidoyl* = imino(phenyl)methyl	C_6H_5-C(=NH)–	P-65.1.7.2.2
benzohydrazido* = 2-benzoylhydrazin-1-yl	C_6H_5-CO-NH-NH–	P-66.3.2.3
benzohydroximoyl = *N*-hydroxybenzenecarboximidoyl* = *N*-hydroxybenzimidoyl = benzenecarbohydroximoyl	C_6H_5-C(=N-OH)–	P-65.1.7.2.2
benzoyl* = benzenecarbonyl = oxo(phenyl)methyl = phenylcarbonyl	C_6H_5-CO–	P-34.2.1.1; P-34.2.2; P-65.1.7.2.1
benzoylamino = benzamido*	C_6H_5-CO-NH–	P-66.1.1.4.3
benzoylazanediyl*	C_6H_5-CO-N<	P-66.1.1.4.4
benzoylazanylidene = benzoylimino*	C_6H_5-CO-N=	P-66.1.1.4.4
2-benzoylhydrazin-1-yl = benzohydrazido*	C_6H_5-CO-NH-NH–	P-66.3.2.3
benzoylimino* = benzoylazanylidene	C_6H_5-CO-N=	P-66.1.1.4.4
benzoyloxy* = (phenylcarbonyl)oxy	C_6H_5-CO-O–	P-65.6.3.2.3
benzyl* = phenylmethyl	C_6H_5-CH_2–	P-29.6.1; P-29.6.2.1
benzylidene* = phenylmethylidene (not benzal)	C_6H_5-CH=	P-29.6.1; P-29.6.2.1
benzylidyne* = phenylmethylidyne	C_6H_5-C≡	P-29.6.1; P-29.6.2.1
benzyloxy* = phenylmethoxy	C_6H_5-CH_2-O–	P-63.2.2.1.1
[1,1′-biphenyl]-4-yl* (not 4-phenylphenyl)		P-29.3.5
bis(acetyloxy)-λ^3-iodanyl* (not diacetoxyiodo)	(CH_3-CO-O)$_2$I–	P-68.5.1
bismuthaniumyl* = bismuthonio = bismuthoniumyl	H_3Bi^+–	P-73.6
bismuthanyl* = bismuthino	H_2Bi–	P-29.3.1; P-68.3.3
λ^5-bismuthanylidene* = bismuthoranylidene	H_3Bi=	P-68.3.3
bismuthino = bismuthanyl*	H_2Bi–	P-29.3.1; P-68.3.3
bismuthonio = bismuthaniumyl* = bismuthoniumyl	H_3Bi^+–	P-73.6
bismuthoniumyl = bismuthaniumyl* = bismuthonio	H_3Bi^+–	P-73.6
bismuthoranylidene = λ^5-bismuthanylidene*	H_3Bi=	P-68.3.3
bis(selanyl)boranyl = diselenoborono*	(HSe)$_2$B–	P-68.1.4.2
bis(silylamino)silyl* (not trisilazan-3-yl)	$SiH_3\text{-}NH\text{-}\overset{\vert}{Si}H\text{-}NH\text{-}SiH_3$	P-29.3.2.2
1,4-bis(sulfanylidene)butane-1,4-diyl = butanebis(thioyl)* = 1,4-dithioxobutane-1,4-diyl	–CS-CH_2-CH_2-CS–	P-65.1.7.4.1; P-65.1.7.4.3

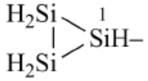
(not dithiosuccinyl)		
bis(sulfanylidene)ethanediyl = dithiooxalyl = ethanebis(thioyl)*	–CS-CS–	P-65.1.7.2.3
bis(sulfanyl)phosphoryl*	$(HS)_2P(O)$–	P-67.1.4.1.1.5
boranediyl* (not borylene; not borylidene; not boranylidene)	HB<	P-68.1.2
boranetriyl* (not borylidyne)	–B<	P-68.1.2
boranuidyl*	H_3B^-–	P-72.6.3
boranyl* (not boryl)	H_2B–	P-29.3.1; P-67.1.4.2; P-68.1.2
(boranylamino)boranyl* (not diborazan-1-yl)	H_2B-NH-BH–	P-68.1.2
boranylidene* (not borylidene)	HB=	P-29.3.1; P-67.1.4.2; P-68.1.2
boranylidyne* (not borylidyne)	B≡	P-29.3.1; P-67.1.4.2
borodiamidoyl: see diaminoboranyl*		
borono* = dihydroxyboranyl	$(HO)_2B$–	P-67.1.4.2; P-68.1.4.2
boryl: see boranyl*		
borylene: see boranediyl*		
borylidene: see boranylidene*		
borylidyne: see boranylidyne*		
bromo*	Br–	P-61.3.1
bromocarbonothioyl = carbonobromidothioyl*	Br-CS–	P-65.2.1.5
bromosyl*	BrO–	P-61.3.2.3
bromyl*	BrO_2–	P-61.3.2.3
butanamido* = butanoylamino = butyramido = butyrylamino	CH_3-$[CH_2]_2$-CO-NH–	P-66.1.1.4.3
butanebis(thioyl)* = 1,4-bis(sulfanylidene)butane-1,4-diyl = 1,4-dithioxobutane-1,4-diyl (not dithiosuccinyl)	–CS-CH_2-CH_2-CS–	P-65.1.7.4.1; P-65.1.7.4.3
butanediimidoyl* = succinimidoyl = 1,4-diiminobutane-1,4-diyl	–C(=NH)-CH_2-CH_2-C(=NH)–	P-65.1.7.3.2
butanedioyl* = succinyl = 1,4-dioxobutane-1,4-diyl	–CO-CH_2-CH_2-CO–	P-65.1.7.3.1; P-65.1.7.4.1
butane-1,1-diyl*	CH_3-CH_2-CH_2-CH<	P-29.3.2.2
butane-1,4-diyl* (not tetramethylene)	–CH_2-CH_2-CH_2-CH_2–	P-29.3.2.2
butanethioyl* = thiobutyryl = 1-sulfanylidenebutyl = 1-thioxobutyl	CH_3-CH_2-CH_2-CS–	P-65.1.7.4.1
butanimidoyl* = butyrimidoyl = 1-iminobutyl	CH_3-CH_2-CH_2-C(=NH)–	P-65.1.7.3.2; P-65.1.7.4.1
butanoyl* = butyryl = 1-oxobutyl	CH_3-CH_2-CH_2-CO–	P-65.1.7.3.1; P-65.1.7.4.1
butanoylamino = butanamido* = butyramido = butyrylamino	CH_3-CH_2-CH_2-CO-NH–	P-66.1.1.4.3
butan-1-yl = butyl*	CH_3-CH_2-CH_2-CH_2–	P-29.3.2.1; P-29.3.2.2
butan-2-yl* = 1-methylpropyl (not *sec*-butyl; not but-2-yl)	CH_3-CH_2-CH(CH_3)–	P-29.3.2.2; P-29.4.1; P-29.6.3
butan-1-ylidene = butylidene*	CH_3-CH_2-CH_2-CH=	P-29.3.2.1; P-29.3.2.2
butan-2-ylidene* = 1-methylpropylidene (not *sec*-butylidene)	CH_3-CH_2-C(CH_3)=	P-29.3.2.2; P-29.4.1; P-29.6.3
butanylidyne = butylidyne*	CH_3-CH_2-CH_2-C≡	P-29.3.2.1; P-29.3.2.2

(butan-2-yl)oxy* = 1-methylpropoxy (not *sec*-butoxy; not *sec*-butyloxy)	$CH_3\text{-}CH_2\text{-}CH(CH_3)\text{-}O–$	P-63.2.2.2
butan-2-yl-3-ylidene*	 $\underset{4}{CH_3}-\overset{\Vert}{\underset{3}{C}}-\overset{\vert}{\underset{2}{CH}}\text{-}\underset{1}{CH_3}$	P-29.3.2.2
butan-3-yl-1-ylidene*	 $\underset{4}{CH_3}\text{-}\overset{\vert}{\underset{3}{CH}}\text{-}\underset{2}{CH_2}\text{-}\underset{1}{CH}=$	P-29.3.2.2
(2*E*)-but-2-enedioyl* = fumaroyl = (2*E*)-1,4-dioxobut-2-ene-1,4-diyl	 $\begin{array}{l} \quad\ \ \overset{2}{HC}\text{-}\overset{1}{CO}– \\ \quad\ \ \ \Vert \\ –\underset{4}{OC}\cdot\underset{3}{CH} \end{array}$	P-65.1.7.3.1; P-65.1.7.4.1
(2*Z*)-but-2-enedioyl* = maleoyl = (2*Z*)-1,4-dioxobut-2-ene-1,4-diyl	 $\begin{array}{l} \overset{2}{HC}\text{-}\overset{1}{CO}– \\ \ \Vert \\ \underset{3}{HC}\text{-}\underset{4}{CO}– \end{array}$	P-65.1.7.3.1; P-65.1.7.4.1
but-2-ene-1,4-diyl*	$–\overset{4}{CH_2}\text{-}\overset{3}{CH}=\overset{2}{CH}\text{-}\overset{1}{CH_2}–$	P-32.1.1
but-2-enoyl* (not crotonyl)	$CH_3\text{-}CH=CH\text{-}CO–$	P-65.1.7.4
but-1-enyl: see but-1-en-1-yl*		
but-1-en-1-yl* (not but-1-enyl)	$CH_3\text{-}CH_2\text{-}CH=CH–$	P-32.1.1
but-2-enyl: see but-2-en-1-yl*		
but-2-en-1-yl* (not but-2-enyl)	$CH_3\text{-}CH=CH\text{-}CH_2–$	P-32.1.1
but-3-en-2-yl* = 1-methylprop-2-en-1-yl	 $\underset{4}{CH_2}=\underset{3}{CH}\cdot\overset{\vert}{\underset{2}{CH}}\text{-}\underset{1}{CH_3}$	P-32.1.1
butoxy* (not butyloxy)	$\overset{4}{CH_3}\text{-}\overset{3}{CH_2}\text{-}\overset{2}{CH_2}\text{-}\overset{1}{CH_2}\text{-}O–$	P-63.2.2.2
sec-butoxy: see (butan-2-yl)oxy*		
tert-butoxy* (unsubstituted) = (2-methylpropan-2-yl)oxy = 1,1-dimethylethoxy (not *tert*-butyloxy)	$(CH_3)_3C\text{-}O–$	P-63.2.2.2
butyl* = butan-1-yl	$CH_3\text{-}CH_2\text{-}CH_2\text{-}CH_2–$	P-29.3.2.1; P-29.3.2.2
but-2-yl: see butan-2-yl*		
sec-butyl: see butan-2-yl*		
tert-butyl* (unsubstituted) = 2-methylpropan-2-yl = 1,1-dimethylethyl	$(CH_3)_3C–$	P-29.4.1; P-29.6.1
butylidene* = butan-1-ylidene	$CH_3\text{-}CH_2\text{-}CH_2\text{-}CH=$	P-29.3.2.1; P-29.3.2.2
sec-butylidene: see butan-2-ylidene*		
butylidyne* = butanylidyne	$CH_3\text{-}CH_2\text{-}CH_2\text{-}C\equiv$	P-29.3.2.1; P-29.3.2.2
butyloxy: see butoxy*		
sec-butyloxy: see (butan-2-yl)oxy*		
tert-butyloxy: see *tert*-butoxy* (unsubstituted)		
butyramido = butanamido* = butyrylamino = butanoylamino	$CH_3\text{-}[CH_2]_2\text{-}CO\text{-}NH–$	P-66.1.1.4.3

butyrimidoyl = butanimidoyl* = 1-iminobutyl	CH_3-CH_2-CH_2-C(=NH)–	P-65.1.7.3.2; P-65.1.7.4.1
butyryl = butanoyl* = 1-oxobutyl	CH_3-CH_2-CH_2-CO–	P-65.1.7.3.1; P-65.1.7.4.1
butyrylamino = butanamido* = butanoylamino = butyramido	CH_3-CH_2-CH_2-CO-NH–	P-66.1.1.4.3
carbamimidamido = carbamimidoylamino* = [amino(imino)methyl]amino = guanidino	H_2N-C(=NH)-NH–	P-66.4.1.2.1.3
carbamimidoyl* = *C*-aminocarbonimidoyl = amino(imino)methyl (not amidino)	H_2N-C(=NH)–	P-65.2.1.5; P-66.4.1.3.1
carbamimidoylamino* = carbamimidamido = [amino(imino)methyl]amino = guanidino	H_2N-C(=NH)-NH–	P-66.4.1.2.1.3
carbamohydrazonoyl* = amino(hydrazinylidene)methyl	H_2N-C(=N-NH_2)–	P-66.4.2.3.2
carbamothioyl* = aminocarbonothioyl = amino(sulfanylidene)methyl (not thiocarbamoyl)	H_2N-CS–	P-65.2.1.5; P-66.1.4.4
carbamothioylamino* = [amino(sulfanylidene)methyl]amino	H_2N-CS-NH–	P-66.1.6.1.3.3
carbamoyl* = aminocarbonyl	H_2N-CO–	P-65.2.1.5; P-66.1.1.4.1.1
carbamoylamino* = (aminocarbonyl)amino (not ureido)	H_2N-CO-NH–	P-66.1.6.1.1.3
carbamoylcarbamoyl* = [(aminocarbonyl)amino]carbonyl	H_2N-CO-NH-CO–	P-66.1.6.1.1.4
carbamoylcarbonyl: see oxamoyl*		
carbamoylformamido: see oxamoylamino*		
carbamoylformyl: see oxamoyl*		
2-carbamoylhydrazin-1-yl* = 2-(aminocarbonyl)hydrazin-1-yl = semicarbazido	H_2N-CO-NH-NH–	P-68.3.1.2.4
carbamoylhydrazinylidene* = semicarbazono	H_2N-CO-NH-N=	P-68.3.1.2.5
carbazimidoyl: see hydrazinecarboximidoyl*		
carbazono: see diazenecarbohydrazido*		
carbazoyl: see hydrazinecarbonyl*		
carboethoxy: see ethoxycarbonyl*		
carbomethoxy: see methoxycarbonyl*		
carbonimidoyl*	–C(=NH)–	P-65.2.1.5
carbonobromidothioyl* = bromocarbonothioyl	Br-CS–	P-65.2.1.5
carbonochloridimidoyl* = *C*-chlorocarbonimidoyl	Cl-C(=NH)–	P-65.2.1.5
carbonochloridoyl* = chlorocarbonyl (not chloroformyl)	Cl-CO–	P-65.2.1.5
carbonocyanidoyl* = cyanocarbonyl = carbononitridoylcarbonyl	NC-CO–	P-65.2.1.5
carbonohydrazidimidoyl = hydrazinecarboximidoyl* = hydrazinyl(imino)methyl = *C*-hydrazinylcarbonimidoyl (not *C*-hydrazinocarbonimidoyl)	H_2N-NH-C(=NH)–	P-66.4.2.3.1
carbonohydrazidoyl = hydrazinecarbonyl* = hydrazinylcarbonyl (not carbazoyl; not hydrazinocarbonyl)	H_2N-NH-CO–	P-66.3.2.1
carbonohydrazonoyl*	–C(=N-NH_2)–	P-65.2.1.5
carbononitridoyl = cyano*	NC–	P-65.2.2; P-66.5.1.1.4
carbononitridoylcarbonyl = carbonocyanidoyl* = cyanocarbonyl	NC-CO–	P-65.2.1.5
carbononitridoyl(disulfanyl) = cyanodisulfanyl* = carbononitridoyldithio (not thiocyanatosulfanyl)	NC-SS–	P-65.2.2
carbononitridoyldithio = cyanodisulfanyl* = carbononitridoyl(disulfanyl)	NC-SS–	P-65.2.2

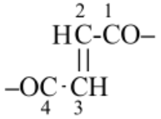
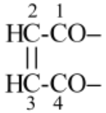
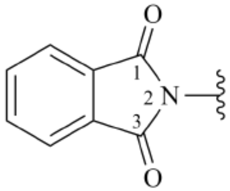
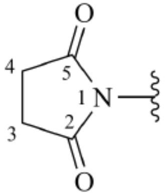
(not thiocyanatosulfanyl)		
carbononitridoyloxy = cyanato*	NC-O–	P-65.2.2
carbononitridoylperoxy = cyanoperoxy*	NC-OO–	P-65.2.2
carbononitridoylselanyl = selenocyanato*	NC-Se–	P-65.2.2
carbononitridoylsulfanyl = thiocyanato* = carbononitridoylthio	NC-S–	P-65.2.2
carbononitridoyltellanyl = tellurocyanato*	NC-Te–	P-65.2.2
carbononitridoylthio = thiocyanato* = carbononitridoylsulfanyl	NC-S–	P-65.2.2
carbonoperoxoyl* = (hydroperoxy)carbonyl (not peroxycarboxy)	(HOO)-CO–	P-65.2.1.5
carbono(thioperoxoyl)* = (thiohydroperoxy)carbonyl	(HOS)-CO– or (HSO)-CO–	P-65.1.5.3; P-65.2.1.7
carbonothioyl* = thiocarbonyl	–CS–	P-65.2.1.5
carbonyl*	–CO–	P-65.2.1.5
carbonylbis(azanediyl)* (not ureylene)	–NH-CO-NH–	P-66.1.6.1.1.3
carboxy*	HOOC–	P-65.1.2.2.3; P-65.2.1.6
carboxyamino*	HOOC-NH–	P-65.2.1.6
carboxycarbonothioyl = carboxymethanethioyl*	HOOC-CS–	P-65.1.7.2.4; P-65.2.1.5
(carboxycarbonothioyl)sulfanyl = (carboxymethanethioyl)sulfanyl*	HOOC-CS-S–	P-65.1.7.2.4; P-65.2.1.5
carboxycarbonyl = oxalo* [not carboxyformyl; not hydroxyl(oxo)acetyl]	HOOC-CO–	P-65.1.2.2.3;P-65.1.7.2.1
(carboxycarbonyl)amino = oxaloamino*	HOOC-CO-NH–	P-65.1.7.2.4
(carboxycarbonyl)oxy = oxalooxy* [not (carboxyformyl)oxy]	HOOC-CO-O–	P-65.1.7.2.4
(carboxycarbonyl)sulfanyl = oxalosulfanyl* = (carboxycarbonyl)thio [not (carboxyformyl)sulfanyl; not (carboxyfomyl)thio]	HOOC-CO-S–	P-65.1.7.2.4
(carboxycarbonyl)thio = oxalosulfanyl* = (carboxycarbonyl)sulfanyl [not (carboxyformyl)sulfanyl; not (carboxyfomyl)thio]	HOOC-CO-S–	P-65.1.7.2.4
carboxyformyl: see oxalo*		
(carboxyformyl)oxy: see oxalooxy*		
(carboxyformyl)sulfanyl: see oxalosulfanyl*		
(carboxyformyl)thio: see oxalosulfanyl*		
carboxylato*	$^-$O-CO–	P-72.6.1
carboxymethanethioyl* = carboxycarbonothioyl	HOOC-CS–	P-65.1.7.2.4; P-65.2.1.5
(carboxymethanethioyl)sulfanyl* = (carboxycarbonothioyl)sulfanyl	HOOC-CS-S–	P-65.1.7.2.4; P-65.2.1.5
3-carboxy-3-oxopropyl (not 2-oxaloethyl)	HOOC-CO-CH_2-CH_2–	P-65.1.2.2.3
carboxyoxy*	HOOC-O–	P-65.2.1.6
(carboxyoxy)carbonyl* [not (carboxyoxy)formyl]	HOOC-O-CO–	P-65.2.3.1.5
(carboxyoxy)formyl: see (carboxyoxy)carbonyl*		
carboxysulfanyl* = carboxythio	HOOC-S–	P-65.2.1.6
carboxythio = carboxysulfanyl*	HOOC-S–	P-65.2.1.6
chloro*	Cl–	P-61.3.1

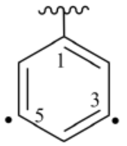
chloroamidophosphoryl: see phosphoramidochloridoyl*		
chloroarsanyl*	ClAsH–	P-67.1.4.1.1.6
chloroboranyl* (not chloroboryl)	ClBH–	P-68.1.4.2
chloroboryl: see chloroboranyl*		
C-chlorocarbonimidoyl = carbonochloridimidoyl*	Cl-C(=NH)–	P-65.2.1.5
chlorocarbonyl = carbonochloridoyl* (not chloroformyl)	Cl-CO–	P-65.2.1.5
chloroformyl: see carbonochloridoyl*		
chlorooxalyl = chloro(oxo)acetyl*	ClCO-CO–	P-65.1.7.2.4
chloro(oxo)acetyl* = chlorooxalyl	ClCO-CO–	P-65.1.7.2.4
chloroso: see chlorosyl*		
chlorosulfinyl*	Cl-S(O)–	P-65.3.2.3; P-67.1.4.4.1
chlorosulfonyl* = sulfurochloridoyl	Cl-SO$_2$–	P-65.3.2.3; P-67.1.4.4.1
(chlorosulfonyl)oxy* = sulfurochloridoyloxy	Cl-SO$_2$-O–	P-65.3.2.3; P-67.1.4.4.2
chlorosyl* (not chloroso)	OCl–	P-61.3.2.3
chloroxy: see chloryl*		
chloryl* (not chloroxy)	O$_2$Cl–	P-61.3.2.3
cinnamoyl = 3-phenylprop-2-enoyl*	C$_6$H$_5$-CH=CH-CO–	P-65.1.7.3.1; P-65.1.7.4.1
crotonyl: see but-2-enoyl*		
cyanato* = carbononitridoyloxy	NC-O–	P-65.2.2
cyano* = carbononitridoyl	NC–	P-65.2.2; P-66.5.1.1.4
cyanocarbonyl = carbonocyanidoyl* = carbononitridoylcarbonyl	NC-CO–	P-65.2.1.5
cyanodisulfanyl* = carbononitridoyl(disulfanyl) = carbononitridoyldithio (not thiocyanatosulfanyl)	NC-SS–	P-65.2.2
cyano(isocyanato)phosphorothioyl = phosphorocyanidoisocyanatidothioyl* = cyano(isocyanato)(thiophosphoryl)	(OCN)(NC)P(S)–	P-67.1.4.1.1.4
cyano(isocyanato)(thiophosphoryl) = phosphorocyanidoisocyanatidothioyl* = cyano(isocyanato)phosphorothioyl	(OCN)(NC)P(S)–	P-67.1.4.1.1.4
cyanoperoxy* = carbononitridoylperoxy	NC-OO–	P-65.2.2
cyanosulfonyl* = sulfurocyanidoyl	NC-SO$_2$–	P-67.1.4.4.1
cyclohexanecarbonyl* = cyclohexylcarbonyl = cyclohexyl(oxo)methyl	C$_6$H$_{11}$-CO–	P-65.1.7.4.2
cyclohexanecarboximidoyl* = cyclohexylcarbonimidoyl = cyclohexyl(imino)methyl (not *C*-cyclohexylcarbonimidoyl)	C$_6$H$_{11}$-C(=NH)–	P-65.1.7.4.2
cyclohexane-1,1-diyl* (not cyclohexanylidene)	C$_6$H$_{10}$<	P-29.3.3
cyclohexane-1,4-diyl* (also 1,1-, 1,2-, and 1,3- isomers) (not 1,4-cyclohexylene)	–C$_6$H$_{10}$–	P-29.3.3
cyclohexanyl = cyclohexyl*	C$_6$H$_{11}$–	P-29.2; P-29.3.3
cyclohexanylidene = cyclohexylidene* (see also: cyclohexane-1,1-diyl)	C$_6$H$_{10}$=	P-29.3.3
cyclohexyl* = cyclohexanyl	C$_6$H$_{11}$–	P-29.2; P-29.3.3

cyclohexylcarbonimidoyl = cyclohexanecarboximidoyl* = cyclohexyl(imino)methyl (not *C*-cyclohexylcarbonimidoyl)	C_6H_{11}-C(=NH)–	P-65.1.7.4.2
C-cyclohexylcarbonimidoyl: see cyclohexanecarboximidoyl*		
cyclohexylcarbonyl = cyclohexanecarbonyl*	C_6H_{11}-CO–	P-65.1.7.4.2
1,4-cyclohexylene: see cyclohexane-1,4-diyl* (also 1,1-, 1,2- and 1,3-isomers)		
cyclohexylidene* = cyclohexanylidene (see also: cyclohexane-1,1-diyl)	C_6H_{10}=	P-29.3.3
cyclohexyl(imino)methyl = cycohexanecarboximidoyl* = cyclohexylcarbonimidoyl (not *C*-cyclohexylcarbonimidoyl)	C_6H_{11}-C(=NH)–	P-65.1.7.4.2
cyclohexyl(oxo)methyl = cyclohexanecarbonyl* = cyclohexylcarbonyl	C_6H_{11}-CO–	P-65.1.7.4.2
cyclopentanecarbohydrazonoyl* = cycopentyl(hydrazinylidene)methyl	C_5H_9-C(=N-NH_2)–	P-65.1.7.4.2
cyclopentanecarboximidoyl* = cyclopentyl(imino)methyl = cyclopentylcarbonimidoyl (not *C*-cyclopentylcarbonimidoyl)	C_5H_9-C(=NH)–	P-65.1.7.4.2
cyclopentylcarbonimidoyl = cyclopentanecarboximidoyl* = cyclopentyl(imino)methyl (not *C*-cyclopentylcarbonimidoyl)	C_5H_9-C(=NH)–	P-65.1.7.4.2
C-cyclopentylcarbonimidoyl: see cyclopentanecarboximidoyl*		
cyclopentyl(hydrazinylidene)methyl = cyclopentanecarbohydrazonoyl*	C_5H_9-C(=N-NH_2)–	P-65.1.7.4.2
cyclopentyl(imino)methyl = cyclopentanecarboximidoyl*	C_5H_9-C(=NH)–	P-65.1.7.4.2
cyclopropanyl = cyclopropyl*	C_3H_5–	P-29.3.3
cyclopropanylidene = cyclopropylidene*	C_3H_4=	P-29.3.3
cyclopropyl* = cyclopropanyl	C_3H_5–	P-29.3.3
cyclopropylidene* = cyclopropanylidene	C_3H_4=	P-29.3.3
cyclotrisilanyl = trisiliranyl*		P-68.2.2
decanedioyl* = 1,10-dioxodecane-1,10-diyl	–CO-[CH_2]$_8$-CO–	P-65.1.7.4.1
decanoyl* = 1-oxodecyl	CH_3-[CH_2]$_8$-CO–	P-65.1.7.4.1
decan-1-yl = decyl*	CH_3-[CH_2]$_8$-CH_2–	P-29.3.2.1; P-29.3.2.2
decan-1-ylidene = decylidene*	CH_3-[CH_2]$_8$-CH=	P-29.3.2.1; P-29.3.2.2
decanylidyne = decylidyne*	CH_3-[CH_2]$_8$-C≡	P-29.3.2.1; P-29.3.2.2
decyl* = decan-1-yl	CH_3-[CH_2]$_8$-CH_2–	P-29.3.2.1; P-29.3.2.2
decylidene* = decan-1-ylidene	CH_3-[CH_2]$_8$-CH=	P-29.3.2.1; P-29.3.2.2
decylidyne* = decanylidyne	CH_3-[CH_2]$_8$-C≡	P-29.3.2.1; P-29.3.2.2
diacetamido: see *N*-acetylacetamido*		
diacetoxyiodo: see bis(acetyloxy)-λ^3-iodanyl*		
diacetylamino = *N*-acetylacetamido* (not diacetylazanyl; not diacetamido)	(CH_3-CO)$_2$N–	P-66.1.2.1
diacetylazanyl: see *N*-acetylacetamido*		
diaminoboranyl* (not borodiamidoyl)	(H_2N)$_2$B–	P-67.1.4.2
(diaminomethylidene)amino*	(H_2N)$_2$C=N–	P-66.4.1.2.1.3

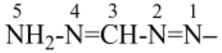
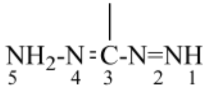
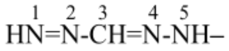
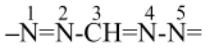
diaminophosphanyl*	$(NH_2)_2P$–	P-67.1.4.1.1.6
diarsanyl*	H_2As-AsH–	P-29.3.2.2
diazane-1,2-diyl = hydrazine-1,2-diyl* (not hydrazo)	–HN-NH–	P-29.3.2.2; P-68.3.1.2.1
diazanediylidene = hydrazinediylidene* (not azino)	=N-N=	P-29.3.2.2; P-68.3.1.2.1
diazanyl = hydrazinyl* (not hydrazino)	H_2N-NH–	P-29.3.2.2; P-68.3.1.2.1
diazanylidene = hydrazinylidene* (not hydrazono)	H_2N-N=	P-29.3.2.2; P-68.3.1.2.1
diazanylidenemethylidene = hydrazinylidenemethylidene* (not hydrazonomethylidene)	H_2N-N=C=	P-65.2.1.8
diazenecarbohydrazido* = 2-(diazenecarbonyl)hydrazin-1-yl (not carbazono)	HN=N-CO-NH-NH–	P-68.3.1.3.4
(diazenecarbonyl)diazenyl*	HN=N-CO-N=N–	P-68.3.1.3.6
2-(diazenecarbonyl)hydrazin-1-yl = diazenecarbohydrazido* (not carbazono)	HN=N-CO-NH-NH–	P-68.3.1.3.4
diazenediyl* = azo	–N=N–	P-32.1.1; P-68.3.1.3.2.1; P-68.3.1.3.2.2
diazenyl*	HN=N–	P-32.1.1; P-68.3.1.3.2.2
diazenyl(hydrazinylidene)methyl = formazan-3-yl*	$H\overset{1}{N}=\overset{2}{N}\text{-}\overset{3}{C}(=\overset{4}{N}\text{-}\overset{5}{N}H_2)$–	P-34.2.1.3; P-68.3.1.3.5.2
(diazenylmethylidene)hydrazinyl = formazan-5-yl*	$H\overset{1}{N}=\overset{2}{N}\text{-}\overset{3}{C}H=\overset{4}{N}\text{-}\overset{5}{N}H$–	P-34.2.1.3; P-68.3.1.3.5.2
diazo*	N_2–	P-61.4
diazoamino: see triaz-1-ene-1,3-diyl*		
diazonio = diazyn-1-ium-1-yl*	$N{\equiv}N^+$–	P-73.6
diazyn-1-ium-1-yl* = diazonio	$N{\equiv}N^+$–	P-73.6
dibismuthane-1,2-diyl*	–BiH-BiH–	P-68.3.3
diborazan-1-yl: see (boranylamino)boranyl*		
diboroxanyl*	H_2B-O-BH–	P-68.1.2
dichloroboranyl* (not dichloroboryl)	Cl_2B–	P-67.1.4.2
dichloroboryl: see dichloroboranyl*		
dichloro-λ^3-iodanyl* (not dichloroiodo)	Cl_2I–	P-68.5.1
dichloroiodo: see dichloro-λ^3-iodanyl*		
dichlorophosphanyl* = dichlorophosphino	Cl_2P–	P-67.1.4.1.1.6; P-68.3.2.3.2.2
dichlorophosphino = dichlorophosphanyl*	Cl_2P–	P-67.1.4.1.1.6; P-68.3.2.3.2.2
dichlorophosphoryl = phosphorodichloridoyl*	$Cl_2P(O)$–	P-67.1.4.1.1.4
dihydroarsoryl = arsinoyl* (not arsinyl)	$H_2As(O)$–	P-67.1.4.1.1.2; P-67.1.4.1.2
dihydronitroryl = azinoyl* (not azinyl)	$H_2N(O)$–	P-67.1.4.1.1.2; P-67.1.4.1.2
dihydrophosphorimidoyl = phosphinimidoyl* = imidophosphinoyl	$H_2P(=NH)$–	P-67.1.4.1.1.4; P-67.1.4.1.2
dihydrophosphorothioyl = phosphinothioyl* = thiophosphinoyl	$H_2P(S)$–	P-67.1.4.1.1.4; P-67.1.4.1.2
dihydrophosphoryl = phosphinoyl* (not phosphinyl)	$H_2P(O)$–	P-67.1.4.1.1.2; P-67.1.4.1.2
dihydrostiborimidoyl = stibinimidoyl* = imidostibinoyl	$H_2Sb(=NH)$–	P-67.1.4.1.1.4; P-67.1.4.1.2
dihydrostiborothioyl = stibinothioyl*	$H_2Sb(S)$–	P-67.1.4.1.1.4; P-67.1.4.1.2

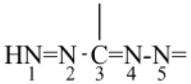
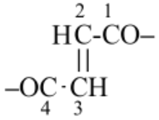
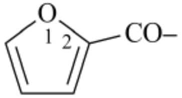
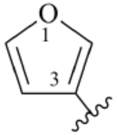
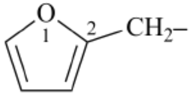
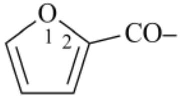
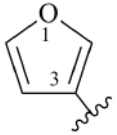
dihydrostiboryl = stibinoyl*	$H_2Sb(O)$–	P-67.1.4.1.1.2; P-67.1.4.1.2
dihydroxyarsoryl = arsono*	$(HO)_2As(O)$–	P-67.1.4.1.1.1
dihydroxyboranyl = borono*	$(HO)_2B$–	P-67.1.4.2; P-68.1.4.2
C,*N*-dihydroxycarbonimidoyl*	HO-C(=N-OH)–	P-65.1.3.3.2
dihydroxy-λ^3-iodanyl* (not dihydroxyiodo)	$(HO)_2I$–	P-68.5.1
dihydroxyiodo: see dihydroxy-λ^3-iodanyl*		
dihydroxynitroryl = azono*	$(HO)_2N(O)$–	P-67.1.4.1.1.1; P-67.1.4.1.1.5
dihydroxyphosphanyl* = dihydroxyphosphino	$(HO)_2P$–	P-67.1.4.1.1.6
dihydroxyphosphino = dihydroxyphosphanyl*	$(HO)_2P$–	P-67.1.4.1.1.6
dihydroxyphosphinothioyl: see dihydroxyphosphorothioyl*		
dihydroxyphosphorothioyl* (not dihydroxyphosphinothioyl)	$(HO)_2P(S)$–	P-67.1.4.1.1.5
dihydroxy(sulfanyl)silyl*	$(HS)(HO)_2Si$–	P-67.1.4.2
1,4-diiminobutane-1,4-diyl = butanediimidoyl* = succinimidoyl	–C(=NH)-CH_2-CH_2-C(=NH)–	P-65.1.7.3.2
diiminoethanediyl = ethanediimidoyl* = oxalimidoyl	–C(=NH)-C(=NH)–	P-65.1.7.2.2
1,3-diiminopropane-1,3-diyl = propanediimidoyl* = malonimidoyl	–C(=NH)-CH_2-C(=NH)–	P-65.1.7.4.1
dimethoxyphosphanyl*	$(CH_3\text{-}O)_2P$–	P-67.1.4.1.1.6
dimethoxyphosphoroselenoyl* = dimethoxy(selenophosphoryl)	$(CH_3\text{-}O)_2P(Se)$–	P-67.1.4.1.1.5
dimethoxyphosphoryl*	$(CH_3\text{-}O)_2P(O)$–	P-67.1.4.1.1.5
(dimethoxyphosphoryl)sulfanyl*	$(CH_3\text{-}O)_2P(O)$-S–	P-67.1.4.1.3
dimethoxy(selenophosphoryl) = dimethoxyphosphoroselenoyl*	$(CH_3\text{-}O)_2P(Se)$–	P-67.1.4.1.1.5
(dimethylamido)phosphoryl = *N*,*N*-dimethylphosphoramidoyl*	$(CH_3)_2N$-P(O)<	P-67.1.4.1.1.4
dimethylammoniumylidene: see *N*-methylmethanaminiumylidene*		
2,3-dimethylanilino* = (2,3-dimethylphenyl)amino (not 2,3-xylidino) (also 2,4-, 2,5-, 2,6-, 3,4-, and 3,5-isomers)	2,3-$(CH_3)_2C_6H_3$-NH–	P-62.2.1.1.2
dimethylazinoyl* (not dimethylnitroryl)	$(CH_3)_2N(O)$–	P-67.1.6
(dimethylboranyl)oxy*	$(CH_3)_2B$-O–	P-68.1.4.2
1,1-dimethylethoxy = (2-methylpropan-2-yl)oxy = *tert*-butoxy* (unsubstituted)	$(CH_3)_3C$-O–	P-63.2.2.2
1,1-dimethylethyl = *tert*-butyl* (unsubstituted) = 2-methylpropan-2-yl	$(CH_3)_3C$–	P-29.4.1; P-29.6.1
dimethylimmonio: see *N*-methylmethanaminiumylidene*		
dimethylnitroryl: see dimethylazinoyl*		
(2,3-dimethylphenyl)amino = 2,3-dimethylanilino* (not 2,3-xylidino) (also 2,4-, 2,5-, 2,6-, 3,4-, and 3,5-isomers)	2,3-$(CH_3)_2C_6H_3$-NH–	P-62.2.1.1.2
dimethylphosphinoselenoyl* = dimethyl(selenophosphinoyl)	$(CH_3)_2P(Se)$–	P-67.1.4.1.1.4
N,*N*-dimethylphosphoramidoyl* = (dimethylamido)phosphoryl	$(CH_3)_2N$-P(O)<	P-67.1.4.1.1.4
1,1-dimethylpropyl = 2-methylbutan-2-yl* (not *tert*-pentyl)	CH_3-CH_2-C$(CH_3)_2$–	P-29.6.3; P-57.1.4
2,2-dimethylpropyl* (not neopentyl)	CH_3-C$(CH_3)_2$-CH_2–	P-57.1.4
dimethyl(selenophosphinoyl) = dimethylphosphinoselenoyl*	$(CH_3)_2P(Se)$–	P-67.1.4.1.1.4

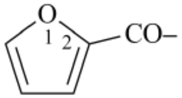
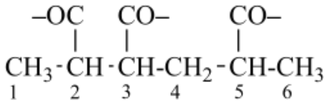
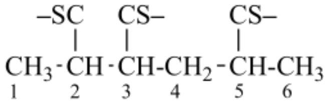
dioxo-λ^5-arsanyl* (not arso)	O_2As–	P-61.6
1,4-dioxobutane-1,4-diyl = butanedioyl* = succinyl	–CO-CH_2-CH_2-CO–	P-65.1.7.3.1; P-65.1.7.4.1
(2*E*)-1,4-dioxobut-2-ene-1,4-diyl = (2*E*)-but-2-enedioyl* = fumaroyl	 $\mathrm{H\overset{2}{C}\text{-}\overset{1}{C}O\text{–}}$ $\mathrm{\text{–}O\underset{4}{C}\cdot\underset{3}{C}H}$	P-65.1.7.3.1; P-65.1.7.4.1
(2*Z*)-1,4-dioxobut-2-ene-1,4-diyl = (2*Z*)-but-2-enedioyl* = maleoyl	 $\mathrm{H\overset{2}{C}\text{-}\overset{1}{C}O\text{–}}$ $\mathrm{H\underset{3}{C}\text{-}\underset{4}{C}O\text{–}}$	P-65.1.7.3.1; P-65.1.7.4.1
1,10-dioxodecane-1,10-diyl = decanedioyl*	–CO-[CH_2]$_8$-CO–	P-65.1.7.4.1
1,3-dioxo-1,3-dihydro-2*H*-isoindol-2-yl* = phthalimido		P-66.2.2
dioxoethanediyl = oxalyl* = ethanedioyl	–CO-CO–	P-65.1.7.2.1
1,6-dioxohexane-1,6-diyl = hexanedioyl* = adipoyl	–CO-[CH_2]$_4$-CO–	P-65.1.7.3.1; P-65.1.7.4.1
1,5-dioxopentane-1,5-diyl = pentanedioyl* = glutaryl	–CO-CH_2-CH_2-CH_2-CO–	P-65.1.7.3.1; P-65.1.7.4.1
dioxo-λ^5-phosphanyl* (not phospho)	O_2P–	P-61.6; P-67.1.4.1.1.6
1,3-dioxopropane-1,3-diyl = propanedioyl* = malonyl	–CO-CH_2-CO–	P-65.1.7.3.1; P-65.1.7.4.1
1,2-dioxopropyl = 2-oxopropanoyl* (not pyruvoyl)	CH_3-CO-CO–	P-65.1.1.2.3; P-65.1.7.4.1
2,5-dioxopyrrolidin-1-yl* = succinimido		P-66.2.2
dioxy: see peroxy*		
diphenylmethyl* (not benzhydryl)	(C_6H_5)$_2$CH–	P-29.6.3
diphosphanyl* (not diphosphino)	H_2P-PH–	P-29.3.2.2; P-45.3.1; P-68.3.2.3.2.2
diphosphino: see diphosphanyl*		
diselanediyl* = diseleno	–Se-Se–	P-63.3.1
diselanyl* = diselenohydroperoxy	HSeSe–	P-63.4.2.2
diseleno = diselanediyl*	–Se-Se–	P-63.3.1
diselenoborono* = bis(selanyl)boranyl	(HSe)$_2$B–	P-68.1.4.2
diselenohydroperoxy = diselanyl*	HSeSe–	P-63.4.2.2
disilane-1,1-diyl*	H_3Si-SiH<	P-29.3.2.2; P-68.2.2
disilanyl* (disilyl)	H_3Si-SiH_2–	P-29.3.2.2; P-68.2.2

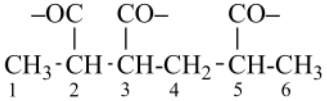
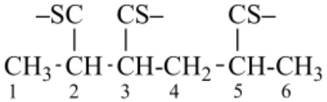
disilazan-1-yl: see (silylamino)silyl*		
disilazan-2-yl: see disilylamino*		
disiloxanyl*	H$_3$Si-O-SiH$_2$–	P-29.3.2.2; P-46.1.3
disilyl: see disilanyl*		
disilylamino* (not disilazan-2-yl)	(SiH$_3$)$_2$N–	P-29.3.2.2; P-68.2.2
disulfanediyl* = dithio	–S-S–	P-63.3.1
disulfanidyl*	$^-$S-S–	P-72.6.3
disulfanyl* = dithiohydroperoxy (not thiosulfeno)	HS-S–	P-63.4.2.2
(disulfanylcarbonyl)oxy* = [(dithiohydroperoxy)carbonyl]oxy	HS-S-CO-O–	P-65.2.1.7
ditellanediyl* = ditelluro	–Te-Te–	P-63.3.1
ditellanyl* = ditellurohydroperoxy	HTe-Te–	P-63.4.2.2
ditelluro = ditellanediyl*	–Te-Te–	P-63.3.1
ditellurohydroperoxy = ditellanyl*	HTe-Te–	P-63.4.2.2
dithio = disulfanediyl*	–S-S–	P-63.3.1
dithiocarbonoperoxoyl* (location of sulfur atoms unknown)	HOS$_2$C–	P-65.1.5.3
dithiocarboxy* = sulfanylcarbonothioyl	HS-CS–	P-65.2.1.6
[(dithiocarboxy)sulfanyl]carbonothioyl* = [sulfanyl(thiocarbonyl)sulfanyl](thiocarbonyl) = [(sulfanylcarbonothioyl)sulfanyl]carbonothioyl {not [(dithiocarboxy)sulfanyl]thioformyl}	HS-CS-S-CS–	P-65.2.3.1.5
[(dithiocarboxy)sulfanyl]thioformyl: see [(dithiocarboxy)sulfanyl]carbonothioyl*		
dithiohydroperoxy = disulfanyl* (not thiosulfeno)	HS-S–	P-63.4.2.2
[(dithiohydroperoxy)carbonyl]oxy = (disulfanylcarbonyl)oxy*	HS-S-CO-O–	P-65.2.1.7
1,2-dithiooxalo: see hydroxy(sulfanylidene)ethanethioyl*		
dithiooxalyl = ethanebis(thioyl)* = bis(sulfanylidene)ethanediyl	–CS-CS–	P-65.1.7.2.3
dithiophthaloyl: see benzene-1,2-dicarbothioyl*		
dithiosuccinyl: see butanebis(thioyl)*		
dithiosulfo* (unspecified)	HO-SS$_2$– or HS-S(=S)(=O)–	P-65.3.2.1
1,4-dithioxobutane-1,4-diyl = butanebis(thioyl)* = 1,4-bis(sulfanylidene)butane-1,4-diyl (not dithiosuccinyl)	–CS-CH$_2$-CH$_2$-CS–	P-65.1.7.4.1; P-65.1.7.4.3
1,1-diyloethyl*	CH$_3$-C$^{2•}$–	P-71.5
3,5-diylophenyl*		P-71.5
dodecanoyl* = 1-oxododecyl	CH$_3$-[CH$_2$]$_{10}$-CO–	P-65.1.7.4.1
dodecan-1-yl = dodecyl*	CH$_3$-[CH$_2$]$_{10}$-CH$_2$–	P-29.3.2.1; P-29.3.2.2
dodecyl* = dodecan-1-yl	CH$_3$-[CH$_2$]$_{10}$-CH$_2$–	P-29.3.2.1; P-29.3.2.2
episeleno = selano* (ring forming)	–Se–	P-25.4.2.1.4; P-63.5

epitelluro = tellano* (ring forming)	–Te–	P-25.4.2.1.4; P-63.5
epithio = sulfano* (ring forming)	–S–	P-25.4.2.1.4; P-63.5
epoxidano: see epoxy* (ring forming)		
epoxy* (ring forming) (not epoxidano)	–O–	P-25.4.2.1.4; P-63.5
ethanebis(thioyl)* = dithiooxalyl = bis(sulfanylidene)ethanediyl	–CS-CS–	P-65.1.7.2.3
ethanediimidoyl* = oxalimidoyl = diiminoethanediyl	–C(=NH)-C(=NH)–	P-65.1.7.2.2
ethanedioyl = oxalyl* = dioxoethanediyl	–CO-CO–	P-65.1.7.2.1
ethanedioylbis(azanediyl) = oxalylbis(azanediyl)*	–HN-CO-CO-NH–	P-66.1.1.4.5.2
ethanedioylbis(azanetriyl) = oxalyldinitrilo* = oxalylbis(azanetriyl) = ethanedioyldinitrilo	>N-CO-CO-N<	P-66.1.1.4.5.2
ethanedioylbis(azanylylidene) = oxalylbis(azanylylidene)*	=N-CO-CO-N=	P-66.1.1.4.5.2
ethanedioyldinitrilo = oxalyldinitrilo* = oxalylbis(azanetriyl) = ethanedioylbis(azanetriyl)	>N-CO-CO-N<	P-66.1.1.4.5.2
ethane-1,1-diyl*	CH$_3$-CH<	P-29.3.2.2
ethane-1,2-diyl* = ethylene	–CH$_2$-CH$_2$–	P-29.3.2.2; P-29.6.2.3
ethane-1,2-diylbis(oxy)* = ethylenebis(oxy) (not ethane-1,2-diyldioxy, not ethylenedioxy)	–O-CH$_2$-CH$_2$-O–	P-63.2.2.1.3
ethane-1,2-diyldioxy: see ethane-1,2-diylbis(oxy)*		
ethanehydrazonamido* = (ethanehydrazonoyl)amino	CH$_3$-C(=N-NH$_2$)-NH–	P-66.4.2.3.5
ethanehydrazonoyl* = acetohydrazonoyl = 1-hydrazinylideneethyl	CH$_3$-C(=N-NH$_2$)–	P-65.1.7.2.2
(ethanehydrazonoyl)amino = ethanehydrazonamido*	CH$_3$-C(=N-NH$_2$)-NH–	P-66.4.2.3.5
ethaneselenoyl* = selenoacetyl = 1-selanylideneethyl	CH$_3$-CSe–	P-65.1.7.2.3
ethanesulfinimidoyl* = *S*-ethylsulfinimidoyl	CH$_3$-CH$_2$-S(=NH)–	P-65.3.2.2.2
ethanesulfinyl* = ethylsulfinyl	CH$_3$-CH$_2$-S(O)–	P-63.6; P-65.3.2.2.2
ethanesulfonimidoyl* = *S*-ethylsulfonimidoyl	CH$_3$-CH$_2$-S(O)(=NH)–	P-65.3.2.2.2
ethanesulfonodiimidamido* = ethanesulfonodiimidoylamino	CH$_3$-CH$_2$-S(=NH)$_2$-NH–	P-66.4.1.3.5
ethanesulfonodiimidoylamino = ethanesulfonodiimidamido*	CH$_3$-CH$_2$-S(=NH)$_2$-NH–	P-66.4.1.3.5
ethanesulfonothioyl* = ethylsulfonothioyl	CH$_3$-CH$_2$-S(O)(S)–	P-65.3.2.2.2
ethanesulfonyl* = ethylsulfonyl	CH$_3$-CH$_2$-SO$_2$–	P-63.6; P-65.3.2.2.2
ethanethioamido* = (ethanethioyl)amino = thioacetamido	CH$_3$-CS-NH–	P-66.1.4.4
ethanethioyl* = thioacetyl = 1-sulfanylideneethyl	CH$_3$-CS–	P-65.1.7.2.3
ethanethioamido* = (ethanethioyl)amino = thioacetamido	CH$_3$-CS-NH–	P-66.1.4.4
(ethanethioyl)amino = ethanethioamido* = thioacetamide	CH$_3$-CS-NH–	P-66.1.4.4
ethanimidamido* = acetimidamido = acetimidoylamino	CH$_3$-C(=NH)-NH–	P-66.4.1.3.5
ethanimidohydrazido* = 2-(ethanimidoyl)hydrazin-1-yl	CH$_3$-C(=NH)-NH-NH–	P-66.4.2.3.6
ethanimidoyl* = acetimidoyl = 1-iminoethyl	CH$_3$-C(=NH)–	P-65.1.7.2.2
2-(ethanimidoyl)hydrazin-1-yl = ethanimidohydrazido*	CH$_3$-C(=NH)-NH-NH–	P-66.4.2.3.6
ethanoyl = acetyl* = 1-oxoethyl	CH$_3$-CO–	P-65.1.7.2.1
ethanyl = ethyl*	CH$_3$-CH$_2$–	P-29.3.2.1; P-29.3.2.2
ethanylidene = ethylidene*	CH$_3$-CH=	P-29.3.2.1; P-29.3.2.2

ethanylidyne = ethylidyne*	CH_3-C≡	P-29.3.2.1; P-29.3.2.2
ethan-1-yl-2-ylidene*	–CH_2-CH=	P-29.3.2.2
ethene-1,2-diyl* (not vinylene)	–CH=CH–	P-32.1.1
ethenyl* = vinyl	CH_2=CH–	P-32.3
ethenylidene* = vinylidene	CH_2=C=	P-32.3
ethoxy* (not ethyloxy)	CH_3-CH_2-O–	P-63.2.2.2
2-ethoxyanilino* = (2-ethoxyphenyl)amino (also 3- and 4-isomers) (not *o*-, *m*-, or *p*-phenetidino)	2-(CH_3-CH_2-O)C_6H_4-NH–	P-62.2.1.1.2
ethoxycarbonyl* (not carboethoxy)	CH_3-CH_2-O-CO–	P-65.6.3.2.3
(2-ethoxyphenyl)amino = 2-ethoxyanilino* (also 3- and 4-isomers) (not *o*-, .*m*-, or *p*-phenetidino)	2-(CH_3-CH_2-O)C_6H_4-NH–	P-62.2.1.1.2
ethyl* = ethanyl	CH_3-CH_2–	P-29.3.2.1; P-29.3.2.2
ethylene = ethane-1,2-diyl*	–CH_2-CH_2–	P-29.6.2.3; P-29.3.2.2
ethylenebis(oxy) = ethane-1,2-diylbis(oxy)* (not ethylenedioxy; not ethane-1,2-diyldioxy)	–O-CH_2CH_2-O–	P-63.2.2.1.3
ethylenedioxy: see ethane-1,2-diylbis(oxy)*		
ethylidene* = ethanylidene	CH_3-CH=	P-29.3.2.1; P-29.3.2.2
ethylidyne* = ethanylidyne	CH_3-C≡	P-29.3.2.1; P-29.3.2.2
ethyloxy: see ethoxy*		
1-ethylpropylidene = pentan-3-ylidene*	(CH_3-CH_2)$_2$C=	P-29.3.2.2; P-29.4.1
ethylstibinoyl*	CH_3-CH_2-SbH(O)–	P-67.1.4.1.1.3
ethylsulfanyl* = ethylthio	CH_3-CH_2-S–	P-63.2.5
S-ethylsulfinimidoyl = ethanesulfinimidoyl*	CH_3-CH_2-S(=NH)–	P-65.3.2.2.2
ethylsulfinyl = ethanesulfinyl*	CH_3-CH_2-S(O)–	P-63.6; P-65.3.2.2.2
S-ethylsulfonimidoyl = ethanesulfonimidoyl*	CH_3-CH_2-S(O)(=NH)–	P-65.3.2.2.2
ethylsulfonothioyl = ethanesulfonothioyl*	CH_3-CH_2-S(O)(S)–	P-65.3.2.2.2
ethylsulfonyl = ethanesulfonyl*	CH_3-CH_2-SO_2–	P-63.6; P-65.3.2.2.2
ethylthio = ethylsulfanyl*	CH_3-CH_2-S–	P-63.2.5
fluoro*	F–	P-61.3.1
fluorosyl*	OF–	P-61.3.2.3
fluoryl*	O_2F–	P-61.3.2.3
formamido* = formylamino	HCO-NH–	P-66.1.1.4.3
formazan-1-yl* = (hydrazinylidenemethyl)diazenyl	 $\overset{5}{NH_2}\text{-}\overset{4}{N}\text{=}\overset{3}{CH}\text{-}\overset{2}{N}\text{=}\overset{1}{N}\text{–}$	P-34.2.1.3; P-68.3.1.3.5.2
formazan-3-yl* = diazenyl(hydrazinylidene)methyl	 $\underset{5}{NH_2}\text{-}\underset{4}{N}\text{=}\underset{3}{\overset{\vert}{C}}\text{-}\underset{2}{N}\text{=}\underset{1}{NH}$	P-34.2.1.3; P-68.3.1.3.5.2
formazan-5-yl* = (diazenylmethylidene)hydrazinyl	 $\overset{1}{HN}\text{=}\overset{2}{N}\text{-}\overset{3}{CH}\text{=}\overset{4}{N}\text{-}\overset{5}{NH}\text{–}$	P-34.2.1.3; P-68.3.1.3.5.2
formazan-1-yl-5-ylidene*	 $\text{–}\overset{1}{N}\text{=}\overset{2}{N}\text{-}\overset{3}{CH}\text{=}\overset{4}{N}\text{-}\overset{5}{N}\text{=}$	P-34.2.1.3; P-68.3.1.3.5.2

formazan-3-yl-5-ylidene*	 $\underset{1}{HN}{=}\underset{2}{N}\cdot\overset{\vert}{\underset{3}{C}}{=}\underset{4}{N}\text{-}\underset{5}{N}{=}$	P-34.2.1.3; P-68.3.1.3.5.2
formimidoyl = methanimidoyl* = iminomethyl	HC(=NH)–	P-65.1.7.2.2
formimidoylamino = methanimidamido* = (iminomethyl)amino	HC(=NH)-NH–	P-66.4.1.3.3
formohydrazido* = 2-formylhydrazin-1-yl	OHC-NH-NH–	P-66.3.5.3
formohydrazonoyl = methanehydrazonoyl* = hydrazinylidenemethyl	$HC(=N\text{-}NH_2)–$	P-65.1.7.2.2
formyl* = methanoyl = oxomethyl	HCO–	P-65.1.7.2.1; P-66.6.1.3
formylamino = formamido*	HCO-NH–	P-66.1.1.4.3
formylazanediyl*	HCO-N<	P-66.1.1.4.4
formylazanylidene = formylimino*	HCO-N=	P-66.1.1.4.4
2-formylhydrazin-1-yl = formohydrazido*	OHC-NH-NH–	P-66.3.5.3
formylimino* = formylazanylidene*	HCO-N=	P-66.1.1.4.4
formyloxy*	HCO-O–	P-65.1.8.3; P-65.6.3.2.3
formylsulfanyl*	HCO-S–	P-65.1.8.3
fulminato: see (λ^2-methylideneamino)oxy*		
fumaroyl = (2*E*)-but-2-enedioyl* = (2*E*)-1,4-dioxobut-2-ene-1,4-diyl	 $\begin{array}{r} \overset{2}{H}\overset{}{C}\text{-}\overset{1}{CO}– \\ \Vert \\ –\underset{4}{OC}\cdot\underset{3}{CH} \end{array}$	P-65.1.7.3.1; P-65.1.7.4.1
furan-2-carbonyl* = 2-furoyl = 2-furylcarbonyl (also 3-isomer)		P-65.1.7.3.1; P-65.1.7.4.2
furan-3-yl* = 3-furyl (also 2-isomer)		P-29.6.2.3; P-57.1.5.3
(furan-2-yl)methyl* (not furfuryl)		P-29.6.3
furfuryl (2-isomer only): see (furan-2-yl)methyl*		
2-furoyl = furan-2-carbonyl* = 2-furylcarbonyl (also 3-isomer)		P-65.1.7.3.1; P-65.1.7.4.2
3-furyl = furan-3-yl* (also 2-isomer)		P-29.6.2.3; P-57.1.5.3

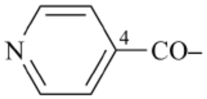
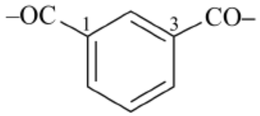
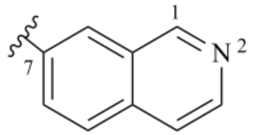
2-furylcarbonyl = furan-2-carbonyl* = 2-furoyl (also 3-isomer)		P-65.1.7.3.1; P-65.1.7.4.2
gallanyl*	H_2Ga–	P-29.3.1; P-68.1.2
germanediyl* (not germylene)	H_2Ge<	P-68.2.2
germanediylidene*	=Ge=	P-68.2.2
germanetetrayl*	>Ge<	P-68.2.2
germanetriyl*	–GeH<	P-68.2.2
germanyl = germyl*	H_3Ge–	P-29.3.1; P-68.2.2
germanylidene = germylidene*	H_2Ge=	P-29.3.1; P-68.2.2
germanylidyne = germylidyne*	HGe≡	P-29.3.1; P-68.2.2
germanylylidene*	–GeH=	P-68.2.2
germyl* = germanyl	H_3Ge–	P-29.3.1; P-68.2.2
germylene: see germanediyl		
germylidene* = germanylidene	H_2Ge=	P-29.3.1; P-68.2.2
germylidyne* = germanylidyne	HGe≡	P-29.3.1; P-68.2.2
glutaryl = pentanedioyl* = 1,5-dioxopentane-1,5-diyl	–CO-CH_2-CH_2-CH_2-CO–	P-65.1.1.2.2; P-65.1.7.3.1
guanidino = carbamimidoylamino* = carbamimidamido = [amino(imino)methyl]amino	H_2N-C(=NH)-NH–	P-66.4.1.2.1.3
heptanoyl* = 1-oxoheptyl	CH_3-$[CH_2]_5$-CO–	P-65.1.7.4.1
heptan-1-yl = heptyl*	CH_3-$[CH_2]_5$-CH_2–	P-29.3.2.1; P-29.3.2.2
heptan-1-ylidene = heptylidene*	CH_3-$[CH_2]_5$-CH=	P-29.3.2.1; P-29.3.2.2
heptanylidyne = heptylidyne*	CH_3-$[CH_2]_5$-C≡	P-29.3.2.1; P-29.3.2.2
heptyl* = heptan-1-yl	CH_3-$[CH_2]_5$-CH_2–	P-29.3.2.1; P-29.3.2.2
heptylidene* = heptan-1-ylidene	CH_3-$[CH_2]_5$-CH=	P-29.3.2.1; P-29.3.2.2
heptylidyne* = heptanylidyne	CH_3-$[CH_2]_5$-C≡	P-29.3.2.1; P-29.3.2.2
hexadecanoyl* = palmitoyl = 1-oxohexadecyl	CH_3-$[CH_2]_{14}$-CO–	P-65.1.7.3.1
hexadecan-1-yl = hexadecyl*	CH_3-$[CH_2]_{14}$-CH_2–	P-29.3.2.1; P-29.3.2.2
hexadecyl* = hexadecan-1-yl	CH_3-$[CH_2]_{14}$-CH_2–	P-29.3.2.1; P-29.3.2.2
hexamethylene: see hexane-1,6-diyl*		
hexanedioyl* = adipoyl = 1,6-dioxohexane-1,6-diyl	–CO-$[CH_2]_4$-CO–	P-65.1.7.3.1; P-65.1.7.4.1
hexane-1,6-diyl* (not hexamethylene)	–CH_2-$[CH_2]_4$-CH_2–	P-29.3.2.2
hexane-2,3,5-tricarbonyl* = hexane-2,3,5-triyltris(oxomethylene) = hexane-2,3,5-triyltricarbonyl	 $\underset{1}{CH_3}\text{-}\underset{2}{\overset{\text{–OC}}{CH}}\text{-}\underset{3}{\overset{\text{CO–}}{CH}}\text{-}\underset{4}{CH_2}\text{-}\underset{5}{\overset{\text{CO–}}{CH}}\text{-}\underset{6}{CH_3}$	P-65.1.7.4.2
hexane-2,3,5-tricarbothioyl* = hexane-2,3,5-triyltris(sulfanylidenemethylene) = hexane-2,3,5-triyltris(thioxomethylene)	 $\underset{1}{CH_3}\text{-}\underset{2}{\overset{\text{–SC}}{CH}}\text{-}\underset{3}{\overset{\text{CS–}}{CH}}\text{-}\underset{4}{CH_2}\text{-}\underset{5}{\overset{\text{CS–}}{CH}}\text{-}\underset{6}{CH_3}$	P-65.1.7.4.2

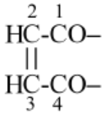
hexane-2,3,5-triyltris(oxomethylene) = hexane-2,3,5-tricarbonyl* = hexane-2,3,5-triyltricarbonyl hexane-2,3,5-triyltricarbonyl = hexane-2,3,5-tricarbonyl* = hexane-2,3,5-triyltris(oxomethylene)	 $\underset{1}{CH_3}\text{-}\underset{2}{\overset{\text{–OC}}{CH}}\text{-}\underset{3}{\overset{\text{CO–}}{CH}}\text{-}\underset{4}{CH_2}\text{-}\underset{5}{\overset{\text{CO–}}{CH}}\text{-}\underset{6}{CH_3}$	P-65.1.7.4.2
hexane-2,3,5-triyltris(thioxomethylene) = hexane-2,3,5-tricarbothioyl* = hexane-2,3,5-triyltris(sulfanylidenemethylene) hexane-2,3,5-triyltris(sulfanylidenemethylene) = hexane-2,3,5-tricarbothioyl* = hexane-2,3,5-triyltris(thioxomethylene)	 $\underset{1}{CH_3}\text{-}\underset{2}{\overset{\text{–SC}}{CH}}\text{-}\underset{3}{\overset{\text{CS–}}{CH}}\text{-}\underset{4}{CH_2}\text{-}\underset{5}{\overset{\text{CS–}}{CH}}\text{-}\underset{6}{CH_3}$	P-65.1.7.4.2
hexanoyl* = 1-oxohexyl	CH_3-$[CH_2]_4$-CO–	P-65.1.7.4.1
hexan-1-yl = hexyl*	CH_3-$[CH_2]_5$–	P-29.3.2.1; P-29.3.2.2
hexan-1-ylidene = hexylidene*	CH_3-$[CH_2]_4$-CH=	P-29.3.2.1; P-29.3.2.2
hexanylidyne = hexylidyne*	CH_3-$[CH_2]_4$-C≡	P-29.3.2.1; P-29.3.2.2
hexyl* = hexan-1-yl	CH_3-$[CH_2]_5$–	P-29.3.2.1; P-29.3.2.2
hexylidene* = hexan-1-ylidene	CH_3-$[CH_2]_4$-CH=	P-29.3.2.1; P-29.3.2.2
hexylidyne* = hexanylidyne	CH_3-$[CH_2]_4$-C≡	P-29.3.2.2; P-29.3.2.1
hydrazi: (not to be used to form heterocycles)		
hydrazidimidophosphoryl = phosphorohydrazidimidoyl*	(H_2N-NH)-P(=NH)<	P-67.1.4.1.1.4
hydrazinecarbohydrazido* = 2-(hydrazinecarbonyl)hydrazin-1-yl = 2-(hydrazinylcarbonyl)hydrazin-1-yl	H_2N-NH-CO-NH-NH–	P-66.3.5.3; P-68.3.1.2.6
hydrazinecarbohydrazonoyl* = *C*-hydrazinylcarbonohydrazonoyl = hydrazinyl(hydrazinylidene)methyl	H_2N-NH-C(=N-NH_2)–	P-66.4.3.4.1
hydrazinecarbonyl* = hydrazinylcarbonyl = carbonohydrazidoyl (not carbazoyl; not hydrazinocarbonyl)	H_2N-NH-CO–	P-66.3.2.1
(hydrazinecarbonyl)diazenyl* = (hydrazinylcarbonyl)diazenyl	H_2N-NH-CO-N=N–	P-68.3.1.3.4
2-(hydrazinecarbonyl)hydrazin-1-yl* = hydrazinecarbohydrazido = 2-(hydrazinylcarbonyl)hydrazin-1-yl	H_2N-NH-CO-NH-NH–	P-66.3.5.3; P-68.3.1.2.6
(hydrazinecarbonyl)hydrazinylidene* = (hydrazinylcarbonyl)hydrazinylidene	H_2N-NH-CO-NH-N=	P-68.3.1.2.6
hydrazinecarboximidoyl* = hydrazinyl(imino)methyl = *C*-hydrazinylcarbonimidoyl = carbonohydrazidimidoyl (not carbazimidoyl; not *C*-hydrazinocarbonimidoyl)	H_2N-NH-CO(=NH)–	P-66.4.2.3.1
hydrazine-1,2-diyl* = diazane-1,2-diyl (not hydrazo)	–NH-NH–	P-29.3.2.2; P-68.3.1.2.1
hydrazinediylidene* = diazanediylidene (not azino)	=N-N=	P-29.3.2.2; P-68.3.1.2.1
hydrazinesulfinyl* = hydrazinylsulfinyl (not hydrazinosulfinyl)	H_2N-NH-S(O)–	P-66.3.2.1
hydrazinesulfonyl* = hydrazinylsulfonyl (not hydrazinosulfonyl)	H_2N-NH-SO_2–	P-66.3.2.1
hydrazino: see hydrazinyl*		
C-hydrazinocarbonimidoyl: see hydrazinecarboximidoyl*		
hydrazinocarbonyl: see hydrazinecarbonyl*		
hydrazinosulfinyl: see hydrazinesulfinyl*		
hydrazinosulfonyl: see hydrazinesulfonyl*		
hydrazinyl* = diazanyl (not hydrazino)	H_2N-NH–	P-29.3.2.2; P-68.3.1.2.1

C-hydrazinylcarbonimidoyl = hydrazinecarboximidoyl* = hydrazinyl(imino)methyl = carbonohydrazidimidoyl (not carbazimidoyl; not *C*-hydrazinocarbonimidoyl)	H_2N-NH-CO(=NH)–	P-66.4.2.3.1
C-hydrazinylcarbonohydrazonoyl = hydrazinecarbohydrazonoyl* = hydrazinyl(hydrazinylidene)methyl	H_2N-NH-C(=N-NH_2)–	P-66.4.3.4.1
hydrazinylcarbonyl = hydrazinecarbonyl* = carbonohydrazidoyl (not carbazoyl; not hydrazinocarbonyl)	H_2N-NH-CO–	P-66.3.2.1
(hydrazinylcarbonyl)diazenyl = (hydrazinecarbonyl)diazenyl*	H_2N-NH-CO-N=N–	P-68.3.1.3.4
2-(hydrazinylcarbonyl)hydrazin-1-yl = hydrazinecarbohydrazido* = 2-(hydrazinecarbonyl)hydrazin-1-yl	H_2N-NH-CO-NH-NH–	P-66.3.5.3; P-68.3.1.2.6
(hydrazinylcarbonyl)hydrazinylidene = (hydrazinecarbonyl)hydrazinylidene*	H_2N-NH-CO-NH-N=	P-68.3.1.2.6
hydrazinyl(hydrazinylidene)methyl = hydrazinecarbohydrazonoyl* = *C*-hydrazinylcarbonohydrazonoyl	H_2N-NH-C(=N-NH_2)–	P-66.4.3.4.1
hydrazinylidene* = diazanylidene (not hydrazono)	H_2N-N=	P-29.3.2.2; P-68.3.1.2.1
1-hydrazinylideneethyl = ethanehydrazonoyl* = acetohydrazonoyl	CH_3-C(=N-NH_2)–	P-65.1.7.2.2
hydrazinylidene(hydroxy)methyl = *C*-hydroxycarbonohydrazonoyl* [not hydrazono(hydoxy)methyl]	HO-C(=N-NH_2)–	P-65.1.3.2.2
hydrazinylidenemethyl = methanehydrazonoyl* = formohydrazonoyl	HC(=N-NH_2)–	P-65.1.7.2.2
(hydrazinylidenemethyl)amino = methanehydrazonamido* = methanehydrazonoylamino	HC(=N-NH_2)-NH–	P-66.4.2.3.3
(hydrazinylidenemethyl)diazenyl = formazan-1-yl*	HC(=N-NH_2)-N=N–	P-34.2.1.3; P-68.3.1.3.5.2
2-(hydrazinylidenemethyl)hydrazin-1-yl = methanehydrazonohydrazido* = 2-(methanehydrazonoyl)hydrazin-1-yl	HC(=N-NH_2)-NH-NH–	P-66.4.3.4.2
hydrazinylidenemethylidene* = diazanylidenemethylidene (not hydrazonomethylidene)	H_2N-N=C=	P-65.2.1.8
1-hydrazinylideneprop-2-en-1-yl = prop-2-enehydrazonoyl* = acrylohydrazonoyl	CH_2=CH-C(=N-NH_2)–	P-65.1.7.3.2
hydrazinyl(imino)methyl = hydrazinecarboximidoyl* = carbonohydrazidimidoyl = *C*-hydrazinylcarbonimidoyl	H_2N-NH-C(=NH)–	P-66.4.2.3.1
hydrazinylsulfinyl = hydrazinesulfinyl* (not hydrazinosulfinyl)	H_2N-NH-S(O)–	P-66.3.2.1
hydrazinylsulfonyl = hydrazinesulfonyl* (not hydrazinosulfonyl)	H_2N-NH-SO_2–	P-66.3.2.1
hydrazo: see hydrazine-1,2-diyl*		
hydrazono: see hydrazinylidene*		
hydrazono(hydroxy)methyl: see *C*-hydroxycarbonohydrazonoyl		
hydrazonomethylidene:: see hydrazinylidenemethylidene*		
hydrazonostiboryl = stiborohydrazonoyl*	–Sb(=N-NH_2)<	P-67.1.4.1.1.4
hydroarsoryl = arsonoyl*	HAs(O)<	P-67.1.4.1.1.2; P-67.1.4.1.2
hydromethoxyboryl: see methoxyboranyl*		
hydronitroryl = azonoyl*	HN(O)<	P-67.1.4.1.1.2; P-67.1.4.1.2
hydroperoxy*	HOO–	P-63.4.2.2
(hydroperoxy)carbonyl = carbonoperoxoyl* (not peroxycarboxy)	(HOO)-CO–	P-65.2.1.5
(hydroperoxy)phosphoryl = phosphoroperoxoyl* = peroxyphosphoryl	(HOO)-P(O)<	P-67.1.4.1.1.4

hydrophosphoryl = phosphonoyl*	HP(O)<	P-67.1.4.1.1.2; P-67.1.4.1.2
hydroseleninyl*	HSe(O)–	P-65.3.2.3
hydroseleno: see selanyl*		
hydrostiboryl = stibonoyl*	HSb(O)<	P-67.1.4.1.1.2; P-67.1.4.1.2
hydrosulfinyl*	HS(O)–	P-65.3.2.3
hydrosulfonyl*	HSO_2–	P-65.3.2.3
hydrotelluro: see tellanyl*		
hydro(thiophosphoryl) = phosphonothioyl*	HP(S)<	P-67.1.4.1.2
hydrotrioxy = trioxidanyl*	HO-O-O–	P-68.4.1.3
hydrotriseleno = triselanyl*	HSe-Se-Se–	P-68.4.1.3
hydrotritelluro = tritellanyl*	HTe-Te-Te–	P-68.4.1.3
hydrotrithio = trisulfanyl*	HS-S-S–	P-68.4.1.3
hydroxy* (not oxidanyl)	HO–	P-63.1.4
N-hydroxyacetimidoyl = *N*-hydroxyethanimidoyl* = acetohydroximoyl	CH_3C(=N-OH)–	P-65.1.7.2.2
hydroxyamino* (not hydroxylamino)	HO-NH–	P-68.3.1.1.1.5
hydroxyarsanyl*	(HO)AsH–	P-67.1.4.1.1.6
hydroxyarsoryl*	(HO)As(O)<	P-67.1.4.1.1.5
hydroxyazanediyl*	HO-N<	P-68.3.1.1.1.5
hydroxyazonoyl*	(HO)HN(O)–	P-67.1.4.1.1.5
N-hydroxybenzenecarboximidoyl* = *N*-hydroxybenzimidoyl = benzenecarbohydroximoyl = benzhydroximoyl	C_6H_5-C(=N-OH)–	P-65.1.7.2.2
N-hydroxybenzimidoyl = *N*-hydroxybenzenecarboximidoyl* = benzenecarbohydroximoyl = benzhydroximoyl	C_6H_5-C(=N-OH)–	P-65.1.7.2.2
hydroxybis(sulfanylidene)ethyl = hydroxy(sulfanylidene)ethanethioyl* (not 1,2-dithiooxalo)	HO-CS-CS–	P-65.1.7.2.4
hydroxyboranyl*	(HO)-HB–	P-67.1.4.2
C-hydroxycarbonimidoyl* = hydroxy(imino)methyl	HO-C(=NH)–	P-35.3.2; P-65.1.3.1.2
(*C*-hydroxycarbonimidoyl)amino* = [hydroxy(imino)methyl]amino (not 1-isoureido)	HO-C(=NH)-NH–	P-66.1.6.1.2.2
C-hydroxycarbonohydrazonoyl* = hydrazinylidene(hydroxy)methyl [not hydrazono(hydroxy)methyl]	HO-C(=N-NH_2)–	P-65.1.3.2.2
hydroxycarbonothioyl*	HO-CS–	P-65.2.1.6
(hydroxycarbonothioyl)carbonyl = hydroxy(thiocarbonyl)carbonyl = hydroxy(sulfanylidene)acetyl* (not 2-thiooxalo; not 2-hydroxy-2-thiooxalyl)	HO-CS-CO–	P-65.1.7.2.4
N-hydroxyethanimidoyl* = *N*-hydroxyacetimidoyl = acetohydroximoyl	CH_3-C(=N-OH)–	P-65.1.7.2.2
hydroxyimino*	HO-N=	P-68.3.1.1.2
hydroxy(imino)methyl = *C*-hydroxycarbonimidoyl*	HO-C(=NH)–	P-35.3.2; P-65.1.3.1.2
[hydroxy(imino)methyl]amino = (*C*-hydroxycarbonimidoyl)amino* (not 1-isoureido)	HO-C(=NH)-NH–	P-66.1.6.1.2.2
hydroxylamino: see hydroxyamino*		

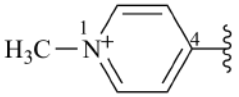
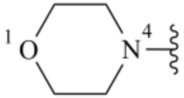
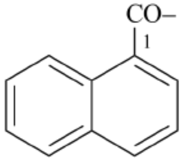
hydroxy(mercapto)phosphoryl: see hydroxy(sulfanyl)phosphoryl*		
hydroxy(methyl)boranyl*	CH_3(HO)B–	P-68.1.4.2
hydroxy(methylphosphonoyl)* = hydroxy(methyl)phosphoryl	CH_3-P(O)(OH)–	P-67.1.4.1.1.5
hydroxy(methyl)phosphoryl = hydroxy(methylphosphonoyl)*	CH_3-P(O)(OH)–	P-67.1.4.1.1.5
hydroxy(oxo)acetyl: see oxalo*		
hydroxy(oxo)-λ^5-arsanylidene*	HO-As(O)=	P-67.1.4.1.1.6
hydroxy(oxo)-λ^5-azanylidene* = *aci*-nitro	HO-N(O)=	P-61.5.3; P-67.1.4.1.1.6; P-67.1.6
hydroxy(oxo)-λ^5-phosphanylidene*	HO-P(O)=	P-67.1.4.1.1.6
hydroxy(oxo)-λ^5-stibanediyl = hydroxystiboryl*	HO-Sb(O)<	P-67.1.4.1.1.5; P-67.1.4.1.1.6
hydroxy(oxo)-λ^5-stibanylidene*	HO-Sb(O)=	P-67.1.4.1.1.6
hydroxyphosphanylidene*	HO-P=	P-67.1.4.1.1.6
hydroxyphosphoryl*	HO-P(O)<	P-67.1.4.1.1.5
hydroxyselanyl* = *OSe*-selenohydroperoxy (not seleneno)	HO-Se–	P-63.4.2.2
(hydroxyselanyl)methyl* = (*OSe*-selenohydroperoxy)methyl	(HO-Se)-CH_2–	P-63.4.2.2
hydroxystibanediyl*	HO-Sb<	P-67.1.4.1.1.6
hydroxystiboryl* = hydroxy(oxo)-λ^5-stibanediyl	HO-Sb(O)<	P-67.1.4.1.1.5; P-67.1.4.1.1.6
hydroxysulfanyl* = *OS*-thiohydroperoxy (not sulfeno; not hydroxythio)	HO-S–	P-63.4.2.2
hydroxy(sulfanyl)boranyl = thioborono*	(HO)(HS)B–	P-68.1.4.2
(hydroxysulfanyl)carbonoselenoyl* = (*OS*-thiohydroperoxy)carbonoselenoyl	(HOS)-C(Se)–	P-65.2.1.7
(hydroxysulfanyl)carbonyl* = (*OS*-thiohydroperoxy)carbonyl	(HOS)-CO–	P-65.1.5.3; P-65.2.1.7
hydroxy(sulfanylidene)acetyl* = (hydroxycarbonothioyl)carbonyl = hydroxy(thiocarbonyl)carbonyl (not 2-thiooxalo; not 2-hydroxy-2-thiooxalyl)	HO-CS-CO–	P-65.1.7.2.4
hydroxy(sulfanylidene)ethanethioyl* = hydroxybis(sulfanylidene)ethyl (not 1,2-dithiooxalo)	HO-CS-CS–	P-65.1.7.2.4
(hydroxysulfanyl)phosphorothioyl* = (*OS*-thiohydroperoxy)phosphorothioyl	(HOS)-P(S)<	P-67.1.4.1.1.5
hydroxy(sulfanyl)phosphoryl* [not hydroxy(mercapto)phosphoryl]	(HO)(HS)P(O)–	P-67.1.4.1.1.5
hydroxysulfonothioyl*	HO-S(O)(S)–	P-65.3.2.3
hydroxytellanyl* = *OTe*-tellurohydroperoxy (not tellureno)	HO-Te–	P-63.4.2.2
hydroxythio: see hydroxysulfanyl*		
hydroxy(thiocarbonyl)carbonyl = hydroxy(sulfanylidene)acetyl* = (hydroxycarbonothioyl)carbonyl (not 2-thiooxalo; not 2-hydroxy-2-thiooxalyl)	HO-CS-CO–	P-65.1.7.2.4
2-hydroxy-2-thiooxalyl: see hydroxy(sulfanylidene)acetyl		
imidoarsoryl = arsorimidoyl*	As(=NH)<	P-67.1.4.1.1.4
imidophosphinoyl = phosphinimidoyl* = dihydrophosphorimidoyl	H_2P(=NH)–	P-67.1.4.1.1.4; P-67.1.4.1.2
imidostibinoyl = stibinimidoyl* = dihydrostiborimidoyl	H_2Sb(=NH)–	P-67.1.4.1.1.2; P-67.1.4.1.2
imino* = azanylidene (see also azanediyl)	HN=	P-35.2.1; P-62.3.1.2
1-iminobutyl = butanimidoyl* = butyrimidoyl	CH_3-CH_2-CH_2-C(=NH)–	P-65.1.7.3.2; P-65.1.7.4.1

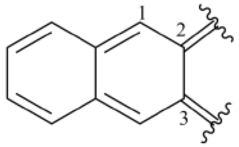
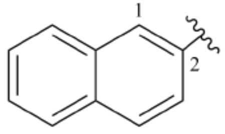
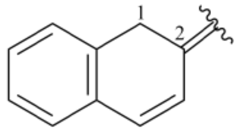
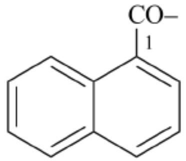
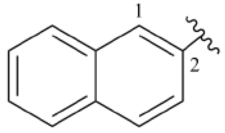
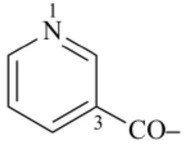
1-iminoethyl = ethanimidoyl* = acetimidoyl	CH_3-C(=NH)–	P-65.1.7.2.2
iminomethyl = methanimidoyl* = formimidoyl	HC(=NH)–	P-65.1.7.2.2
(iminomethyl)amino = methanimidamido* = formimidoylamino	HN=CH-NH–	P-66.4.1.3.3
iminomethylidene*	HN=C=	P-65.2.1.8
imino(phenyl)methyl = benzenecarboximidoyl* = benzimidoyl	C_6H_5-C(=NH)–	P-65.1.7.2.2
1-iminopropyl = propanimidoyl* = propionimidoyl	CH_3-CH_2-C(=NH)–	P-65.1.7.3.2; P-65.1.7.4.1
1-imino-2-selanylideneethane-1,2-diyl*	–C(=NH)-C(Se)–	P-65.1.7.5
[imino(sulfanyl)methyl]amino = (*C*-sulfanylcarbonimidoyl)amino*	HS-C(=NH)-NH–	P-66.1.6.1.3.3
indiganyl*	H_2In–	P-29.3.1; P-68.1.2
iodoso: see iodosyl*		
iodosyl* (not iodoso)	OI–	P-61.3.2.3
iodyl*	O_2I–	P-61.3.2.3
isobutoxy: see 2-methylpropoxy*		
isobutyl: see 2-methylpropyl*		
isocyanato*	OCN–	P-61.8
isocyano*	CN–	P-61.9
isofulminato: see (oxo-λ^5-azanylidyne)methyl*		
isonicotinoyl = pyridine-4-carbonyl* = 4-pyridylcarbonyl = oxo(pyridine-4-yl)methyl		P-65.1.7.3.1; P-65.1.7.4.2
isopentyl: see 3-methylbutyl*		
isophthaloyl = benzene-1,3-dicarbonyl* = 1,3-phenylenedicarbonyl = 1,3-phenlenebis(oxomethylene)		P-65.1.7.3.1; P-65.1.7.4.2
isopropenyl = prop-1-en-2-yl* = 1-methylethen-1-yl	CH_2=C(CH_3)–	P-32.1.1; P-32.3
isopropoxy = (propan-2-yl)oxy* = 1-methylethoxy	$(CH_3)_2$CH-O–	P-63.2.2.2
isopropyl = propan-2-yl* = 1-methylethyl	$(CH_3)_2$CH–	P-29.3.2.2; P-29.4.1; P-29.6.2.2
isopropylidene = propan-2-ylidene* = 1-methylethylidene	$(CH_3)_2$C=	P-29.3.2.2; P-29.4.1; P-29.6.2.2
isoquinolin-7-yl* = 7-isoquinolyl (also 1-, 3-, 4-, 5-, 6- and 8-isomers) 7-isoquinolyl = isoquinolin-7-yl* (also 1-, 3-, 4-, 5-, 6- and 8-isomers)		P-29.3.4.1; P-57.1.5.3
isoselenocyanato*	SeCN–	P-61.8
isotellurocyanato*	TeCN–	P-61.8
isothiocyanato*	SCN–	P-61.8
isothiocyanatosulfonothioyl* = sulfur(isothiocyanatido)thioyl	(SCN)-S(O)(S)–	P-67.1.4.4.1
isothiocyanatosulfonyl* = sulfur(isothiocyanatidoyl)	(SCN)-SO_2–	P-67.1.4.4.1

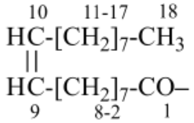
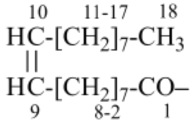
1-isoureido: see (*C*-hydroxycarbonimidoyl)amino*		
3-isoureido: see [amino(hydroxy)methylidene]amino*		
keto (not to be used): see oxo*		
maleoyl = (2*Z*)-but-2-enedioyl* = (2*Z*)-1,4-dioxobut-2-ene-1,4-diyl	 $\overset{2}{\mathrm{HC}}\text{-}\overset{1}{\mathrm{CO}}\text{–} = \underset{3}{\mathrm{HC}}\text{-}\underset{4}{\mathrm{CO}}\text{–}$	P-65.1.7.3.1; P-65.1.7.4.1
malonimidoyl = propanediimidoyl* = 1,3-diiminopropane-1,3-diyl	–C(=NH)-CH$_2$-C(=NH)–	P-65.1.7.4.1
malonyl = propanedioyl* = 1,3-dioxopropane-1,3-diyl	–CO-CH$_2$-CO–	P-65.1.7.3.1; P-65.1.7.4.1
mercapto: see sulfanyl*		
mercaptocarbonyl: see sulfanylcarbonyl*		
mercaptooxy: see sulfanyloxy*		
methacryloyl = 2-methylprop-2-enoyl* = 2-methyl-1-oxoprop-2-en-1-yl	CH$_2$=C(CH$_3$)-CO–	P-65.1.7.3.1; P-65.1.7.4.1
methanediyl: see methylene*		
methanehydrazonamido* = methanehydrazonoylamino = (hydrazinylidenemethyl)amino	HC(=N-NH$_2$)-NH–	P-66.4.2.3.3
methanehydrazonohydrazido* = 2-(methanehydrazonoyl)hydrazin-1-yl = 2-(hydrazinylidenemethyl)hydrazin-1-yl	HC(=N-NH$_2$)-NH-NH–	P-66.4.3.4.2
methanehydrazonoyl* = formohydrazonoyl = hydrazinylidenemethyl	HC(=N-NH$_2$)–	P-65.1.7.2.2
methanehydrazonoylamino = methanehydrazonamido* = (hydrazinylidenemethyl)amino	HC(=N-NH$_2$)-NH–	P-66.4.2.3.3
2-(methanehydrazonoyl)hydrazin-1-yl = methanehydrazonohydrazido* = 2-(hydrazinylidenemethyl)hydrazin-1-yl	CH(=N-NH$_2$)-NH-NH–	P-66.4.3.4.2
methaneseleninyl* = methylseleninyl	CH$_3$-Se(O)–	P-65.3.2.2.2
methaneselenonyl* = methylselenonyl	CH$_3$-SeO$_2$–	P-65.3.2.2.2
methaneselenoyl* = selenoformyl = selanylidenemethyl	HC(Se)–	P-65.1.7.2.3; P-66.6.3
methanesulfinamido* = (methanesulfinyl)amino	CH$_3$-S(O)-NH–	P-66.1.1.4.3
methanesulfinimidoyl* = *S*-methylsulfinimidoyl	CH$_3$-S(=NH)–	P-65.3.2.2.2
methanesulfinyl* = methylsulfinyl	CH$_3$-S(O)–	P-65.3.2.2.2
(methanesulfinyl)amino = methanesulfinamido*	CH$_3$-S(O)-NH–	P-66.1.1.4.3
methanesulfonamido* = (methanesulfonyl)amino	CH$_3$-SO$_2$-NH–	P-66.1.1.4.3
methanesulfonimidoyl* = *S*-methylsulfonimidoyl	CH$_3$-S(=NH)(O)–	P-65.3.2.2.2
methanesulfonyl* = methylsulfonyl	CH$_3$-SO$_2$–	P-65.3.2.2.2
(methanesulfonyl)amino = methanesulfonamido*	CH$_3$-SO$_2$-NH–	P-66.1.1.4.3
(methanesulfonyl)azanylidene = (methanesulfonyl)imino* = (methylsulfonyl)imino	CH$_3$-SO$_2$-N=	
(methanesulfonyl)imino* = (methylsulfonyl)imino = (methanesulfonyl)azanylidene	CH$_3$-SO$_2$-N=	P-66.1.1.4.4
methanetelluroyl* = telluroformyl = tellanylidenemethyl	HC(Te)–	P-65.1.7.2.3; P-66.6.3
methanetetrayl*	>C<	P-29.3.1
methanethioamido* = (methanethioyl)amino = thioformamido	HCS-NH–	P-66.1.4.4
methanethioyl* = thioformyl = sulfanylidenemethyl	HCS–	P-65.1.7.2.3; P-66.6.3

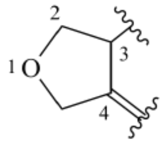
(methanethioyl)amino = methanethioamido* = thioformamido	HCS-NH–	P-66.1.4.4
methanetriyl*	–CH<	P-29.3.1
methanidyl*	H_2C^{-}–	P-72.6.3
methanimidamido* = (iminomethyl)amino = formimidoylamino	HC(=NH)-NH–	P-66.4.1.3.3
methanimidoyl* = formimidoyl = iminomethyl	HC(=NH)–	P-65.1.7.2.2
methanoyl = formyl* = oxomethyl	HCO–	P-65.1.7.2.1; P-66.6.1.3
methanyl = methyl*	CH_3–	P-29.3.1
methanylidene = methylidene*	CH_2=	P-29.3.1
methanylidyne = methylidyne*	CH≡	P-29.3.1
methanylylidene*	–CH=	P-29.3.1
methoxy* (not methyloxy)	CH_3-O–	P-63.2.2.2
2-methoxyanilino* = (2-methoxyphenyl)amino (also 3- and 4-methoxy isomers) (not 2-anisidino; not *o*-anisidino)	2-(CH_3-O)-C_6H_4-NH–	P-62.2.1.1.2
methoxyboranyl* (not hydromethoxyboryl)	CH_3-O-BH–	P-67.1.4.2
methoxyboranylidene*	CH_3-O-B=	P-67.1.4.1.1.6
C-methoxycarbonimidoyl*	CH_3-O-C(=NH)–	P-65.2.1.5
methoxycarbonothioyl* = methoxythiocarbonyl	CH_3-O-CS–	P-65.2.1.5
methoxycarbonyl* (not carbomethoxy)	CH_3-O-CO–	P-65.6.3.2.3
methoxy(isocyanato)phosphoryl*	(CH_3-O)(OCN)P(O)–	P-67.1.4.1.1.5
methoxy(oxo)-λ^5-arsanylidene*	CH_3-O-As(O)=	P-67.1.4.1.1.6
(2-methoxyphenyl)amino = 2-methoxyanilino* (also *m* = 3- and *p* = 4-isomers)	2-(CH_3-O)-C_6H_4-NH–	P-62.2.1.1.2
methoxysulfanyl* (not methoxythio)	CH_3-O-S–	P-63.3.2
S-methoxysulfinimidoyl*	CH_3-O-S(=NH)–	P-65.3.2.3
(methoxysulfinyl)oxy*	CH_3-O-S(O)-O–	P-67.1.4.4.2
methoxysulfonyl* = methoxysulfuryl	CH_3-O-SO_2–	P-65.3.2.3; P-67.1.4.4.1
(methoxysulfonyl)amino*	CH_3-O-S(O)$_2$-NH–	P-67.1.4.4.2
methoxysulfuryl = methoxysulfonyl*	CH_3-O-SO_2–	P-65.3.2.3; P-67.1.4.4.1
methoxythio: see methoxysulfanyl*		
methoxythiocarbonyl = methoxycarbonothioyl*	CH_3-O-CS–	P-65.2.1.5
methyl* = methanyl	CH_3–	P-29.3.1
(methylamino)sulfinyl*	CH_3-NH-S(O)–	P-66.1.1.4.2
2-methylanilino* = (2-methylphenyl)amino (not *o*-toluidino; not 2-toluidino) (also 3- and 4-isomers)	2-CH_3-C_6H_4-NH–	P-62.2.1.1.2
(methylboranyl)amino*	CH_3-BH-NH–	P-68.1.4.2
2-methylbutan-2-yl* = 1,1-dimethylpropyl (not *tert*-pentyl)	CH_3-CH_2-C(CH_3)$_2$–	P-29.4.1; P-29.6.3; P-57.1.4
1-methylbutyl = pentan-2-yl*	CH_3-CH_2-CH_2-CH(CH_3)–	P-29.3.2.2; P-29.4.1
2-methylbutyl*	CH_3-CH_2-CH(CH_3)-CH_2–	P-29.4.1

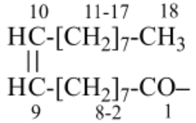
3-methylbutyl* (not isopentyl)	$(CH_3)_2CH$-CH_2-CH_2–	P-29.4.1; P-29.6.3
methyldioxy: see methylperoxy*		
methyldiselanyl* = methyldiseleno	CH_3-Se-Se–	P-63.3.1
methyldiseleno = methyldiselanyl*	CH_3-Se-Se–	P-63.3.1
methyldisulfanyl* = methyldithio	CH_3-S-S–	P-63.3.1
methylditellanyl* = methylditelluro	CH_3-Te-Te–	P-63.3.1
methylditelluro = methylditellanyl*	CH_3-Te-Te–	P-63.3.1
methyldithio = methyldisulfanyl*	CH_3-S-S–	P-63.3.1
methylene* (not methanediyl)	–CH_2–	P-29.6.1
methylenebis(oxy)* (not methylenedioxy)	–O-CH_2-O–	P-63.2.2.1.3
methylenebis(sulfanediyl)* = methylenebis(thio)	–S-CH_2-S–	P-63.2.2.1.3
methylenebis(thio) = methylenebis(sulfanediyl)*	–S-CH_2-S–	P-63.2.2.1.3
methylenedioxy: see methylenebis(oxy)*		
1-methylethane-1,2-diyl = propane-1,2-diyl* (not propylene)	–CH_2-$CH(CH_3)$–	P-29.3.2.2
1-methylethen-1-yl = prop-1-en-2-yl* = isopropenyl	CH_2=$C(CH_3)$–	P-32.1.1; P-32.3
1-methylethoxy = (propan-2-yl)oxy* = isopropoxy	$(CH_3)_2CH$-O–	P-63.2.2.2
1-methylethyl = propan-2-yl* = isopropyl	$(CH_3)_2CH$–	P-29.3.2.2; P-29.4.1; P-29.6.2.2
1-methylethylidene = propan-2-ylidene* = isopropylidene	$(CH_3)_2C$=	P-29.3.2.2; P-29.4.1; P-29.6.2.2
methylidene* = methanylidene	CH_2=	P-29.3.1
(λ^2-methylideneamino)oxy* (not fulminato)	C=N-O–	P-61.10
methylidyne* = methanylidyne	CH≡	P-29.3.1
N-methylmethanaminiumylidene* (not dimethylammoniumylidene; not dimethylimmonio)	$(CH_3)_2N^+$=	P-73.6
2-methyl-1-oxoprop-2-en-1-yl = 2-methylprop-2-enoyl* = methacryloyl	CH_2=$C(CH_3)$-CO–	P-65.1.7.3.1; P-65.1.7.4.1
methyloxy = methoxy*		
methylperoxy* (not methyldioxy)	CH_3-OO–	P-63.3.1
2-methylphenyl* = *o*-toly (also *m*- = 3- and *p*- = 4-isomers)	2-CH_3-C_6H_4–	P-29.6.2.3; P-57.1.5.3
(2-methylphenyl)amino = 2-methylanilino* (not *o*-toluidino; not 2-toluidino) (also 3- and 4-isomers)	2-CH_3-C_6H_4-NH–	P-62.2.1.1.2
methyl(phenyl)arsinoyl*	$(C_6H_5)(CH_3)As(O)$–	P-67.1.4.1.1.3
methylphosphonoyl*	CH_3-P(O)<	P-67.1.4.1.1.3
2-methylpropan-2-yl = *tert*-butyl* (unsubstituted) = 1,1-dimethylethyl	$(CH_3)_3C$–	P-29.4.1; P-29.6.1
2-methylpropan-2-ylium-1-yl*	CH_3-$C^+(CH_3)$-CH_2–	P-73.6
(2-methylpropan-2-yl)oxy = *tert*-butoxy* (unsubstituted) = 1,1-dimethylethoxy	$(CH_3)_3C$-O–	P-63.2.2.2
2-methylprop-2-enoyl* = methacryloyl = 2-methyl-1-oxoprop-2-en-1-yl	CH_2=$C(CH_3)$-CO–	P-65.1.7.3.1; P-65.1.7.4.1
1-methylprop-2-en-1-yl = but-3-en-2-yl*	CH_2=CH-$CH(CH_3)$–	P-32.1.1
1-methylpropoxy = (butan-2-yl)oxy* (not *sec*-butoxy; not *sec*-butyloxy)	CH_3-CH_2-$CH(CH_3)$-O–	P-63.2.2.2
2-methylpropoxy* (not isobutoxy)	CH_3-$CH(CH_3)$-CH_2-O–	P-63.2.2.2

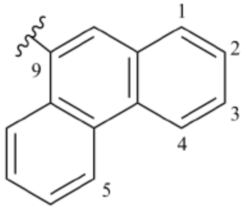
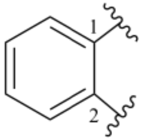
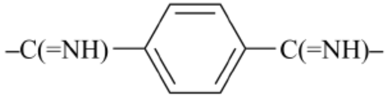
1-methylpropyl = butan-2-yl* (not *sec*-butyl; not but-2-yl)	$\mathrm{CH_3{-}CH_2{-}CH(CH_3){-}}$	P-29.3.2.2; P-29.4.1; P-29.6.3
2-methylpropyl* (not isobutyl)	$\mathrm{CH_3{-}CH(CH_3){-}CH_2{-}}$	P-29.6.3; P-57.1.4
1-methylpropylidene = butan-2-ylidene* (not *sec*-butylidene)	$\mathrm{CH_3{-}CH_2{-}C(CH_3){=}}$	P-29.3.2.2; P-29.4.1; P-29.6.3
1-methylpyridin-1-ium-4-yl*		P-73.6
methylselanyl* = methylseleno	$\mathrm{CH_3{-}Se{-}}$	P-63.2.2.1.2; P-63.2.5
methylseleninyl = methaneseleninyl*	$\mathrm{CH_3{-}Se(O){-}}$	P-65.3.2.2.2
methylseleno = methylselanyl*	$\mathrm{CH_3{-}Se{-}}$	P-63.2.2.1.2; P-63.2.5
methylselenonyl = methaneselenonyl*	$\mathrm{CH_3{-}SeO_2{-}}$	P-65.3.2.2.2
methylsulfaniumdiyl* = methylsulfoniumdiyl	$\mathrm{CH_3{-}S^{+}{<}}$	P-73.6
methylsulfanyl* = methylthio	$\mathrm{CH_3{-}S{-}}$	P-63.2.2.1.2; P-63.2.5
(methylsulfanyl)oxy* [not (methylthio)oxy]	$\mathrm{CH_3{-}S{-}O{-}}$	P-63.3.2
(methylsulfanyl)sulfonyl* = (methylthio)sulfonyl	$\mathrm{CH_3{-}S{-}SO_2{-}}$	P-65.3.2.3; P-65.6.3.2.3
S-methylsulfinimidoyl = methanesulfinimidoyl*	$\mathrm{CH_3{-}S({=}NH){-}}$	P-65.3.2.2.2
methylsulfinyl = methanesulfinyl*	$\mathrm{CH_3{-}S(O){-}}$	P-65.3.2.2.2
S-methylsulfonimidoyl = methanesulfonimidoyl*	$\mathrm{CH_3{-}S({=}NH)(O){-}}$	P-65.3.2.2.2
methylsulfoniumdiyl = methylsulfaniumdiyl*	$\mathrm{CH_3{-}S^{+}{<}}$	P-73.6
methylsulfonyl = methanesulfonyl*	$\mathrm{CH_3{-}SO_2{-}}$	P-65.3.2.2.2
(methylsulfonyl)imino = (methanesulfonyl)imino* [not (methanesulfonyl)azanylidene]	$\mathrm{CH_3{-}SO_2{-}N{=}}$	P-66.1.1.4.4
methyltellanyl* = methyltelluro	$\mathrm{CH_3{-}Te{-}}$	P-63.2.5
methyltelluro = methyltellanyl*	$\mathrm{CH_3{-}Te{-}}$	P-63.2.5
1-methyltetrasilan-1-yl*	$\mathrm{SiH_3{-}SiH_2{-}SiH_2{-}SiH(CH_3){-}}$	P-29.4.1
methylthio = methylsulfanyl*	$\mathrm{CH_3{-}S{-}}$	P-63.2.2.1.2; P-63.2.5
(methylthio)oxy: see (methylsulfanyl)oxy*		
(methylthio)sulfonyl = (methylsulfanyl)sulfonyl*	$\mathrm{CH_3{-}S{-}SO_2{-}}$	P-65.3.2.3; P-65.6.3.2.3
methyltrisulfanyl* = methyltrithio	$\mathrm{CH_3{-}S{-}S{-}S{-}}$	P-68.4.1.3
methyltrithio = methyltrisulfanyl*	$\mathrm{CH_3{-}S{-}S{-}S{-}}$	P-68.4.1.3
morpholino: see morpholin-4-yl*		
morpholin-4-yl* (not morpholino)		P-29.3.3; P-29.6.2.3; P-64.7.1
naphthalene-1-carbonyl* = 1-naphthoyl = 1-naphthylcarbonyl = naphthalen-1-yl(oxo)methyl (also 2-isomer)		P-65.1.7.3.1; P-65.1.7.4.2

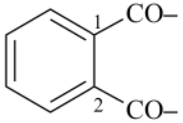
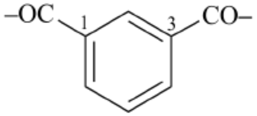
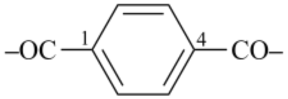
naphthalene-2,3-diylidene*		P-29.3.4.1
naphthalen-2-yl* = 2-naphthyl (also 1-isomer)		P-29.3.4.1; P-29.6.2.3; P-57.1.5.3
naphthalen-1-yl(oxo)methyl = naphthalene-1-carbonyl* = 1-naphthoyl = 1-naphthylcarbonyl (also 2-isomer)	1-$C_{10}H_7$-CO–	P-65.1.7.3.1; P-65.1.7.4.2
naphthalen-2(1*H*)-ylidene* [also 1(2*H*)-isomer]		P-29.3.4.1
1-naphthoyl = naphthalene-1-carbonyl* = 1-naphthylcarbonyl = naphthalen-1-yl(oxo)methyl (also 2-isomer)		P-65.1.7.3.1; P-65.1.7.4.2
2-naphthyl = naphthalen-2-yl* (also 1-isomer)		P-29.3.4.1; P-29.6.2.3
1-naphthylcarbonyl = naphthalene-1-carbonyl* = 1-naphthoyl = naphthalen-1-yl(oxo)methyl (also 2-isomer)	1-$C_{10}H_7$-CO–	P-65.1.7.3.1; P-65.1.7.4.2; P-57.1.5.3
neopentyl: see 2,2-dimethylpropyl*		
nicotinoyl = pyridine-3-carbonyl* = 3-pyridylcarbonyl = oxo(pyridin-3-yl)methyl		P-65.1.7.3.1; P-65.6.3.2.3
nitramido* = nitroamino	O_2N-NH–	P-67.1.4.3.2
nitridophosphoryl = phosphoronitridoyl*	N≡P<	P-67.1.4.1.1.4
nitridostiboryl = stiboronitridoyl*	N≡Sb<	P-67.1.4.1.1.4
nitrilo* = azanetriyl (not azanylidyne; not azanylylidene)	–N<	P-35.2.1; P-62.2.5.1
nitro*	O_2N–	P-61.5.1
aci-nitro = hydroxy(oxo)-λ^5-azanylidene*	HO-N(O)=	P-61.5.3; P-67.1.4.1.1.6; P-67.1.6
nitroamino = nitramido*	O_2N-NH–	P-67.1.4.3.2
nitroazanediyl*	O_2N-N<	P-67.1.4.3.2
1-nitrohydrazin-1-yl*	H_2N-N(NO_2)–	P-67.1.4.3.3

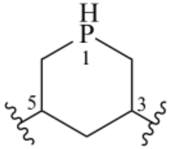
2-nitrohydrazin-1-yl*	$\mathrm{O_2N\text{-}NH\text{-}NH}$–	P-67.1.4.3.3
nitroimino*	$\mathrm{O_2N\text{-}N{=}}$	P-67.1.4.3.2
nitrooxy*	$\mathrm{O_2N\text{-}O}$–	P-67.1.4.3.1
nitroryl* (not azoryl)	–N(O)<	P-67.1.4.1.1.2
nitroso*	O=N–	P-61.5.1
nitrosoamino*	ON-NH–	P-67.1.4.3.2
nitrosohydrazinylidene*	ON-NH-N=	P-67.1.4.3.3
nitrosooxy*	ON-O–	P-67.1.4.3.1
nitrososelanyl*	ON-Se–	P-67.1.4.3.1
nitrosulfanyl*	$\mathrm{O_2N\text{-}S}$–	P-67.1.4.3.1
nonanoyl* = 1-oxononyl	$\mathrm{CH_3\text{-}[CH_2]_7\text{-}CO}$–	P-65.1.7.4.1
nonan-1-yl = nonyl*	$\mathrm{CH_3\text{-}[CH_2]_7\text{-}CH_2}$–	P-29.3.2.1; P-29.3.2.2
nonan-1-ylidene = nonylidene*	$\mathrm{CH_3\text{-}[CH_2]_7\text{-}CH{=}}$	P-29.3.2.1; P-29.3.2.2;
nonanylidyne = nonylidyne*	$\mathrm{CH_3\text{-}[CH_2]_7\text{-}C{\equiv}}$	P-29.3.2.1; P-29.3.2.2
nonyl* = nonan-1-yl	$\mathrm{CH_3\text{-}[CH_2]_7\text{-}CH_2}$–	P-29.3.2.1; P-29.3.2.2
nonylidene* = nonan-1-ylidene	$\mathrm{CH_3\text{-}[CH_2]_7\text{-}CH{=}}$	P-29.3.2.1; P-29.3.2.2
nonylidyne* = nonanylidyne	$\mathrm{CH_3\text{-}[CH_2]_7\text{-}C{\equiv}}$	P-29.3.2.1; P-29.3.2.2
octadecanoyl* = stearoyl = 1-oxooctadecyl	$\mathrm{CH_3\text{-}[CH_2]_{16}\text{-}CO}$–	P-65.1.7.3.1; P-65.1.7.4.1
octadecan-1-yl = octadecyl*	$\mathrm{CH_3\text{-}[CH_2]_{17}}$–	P-29.3.2.1; P-29.3.2.2
(9*Z*)-octadec-9-enoyl* = oleoyl = (9*Z*)-1-oxooctadec-9-en-1-yl	 $\begin{array}{l}\overset{10}{\mathrm{HC}}\text{-}\overset{11\text{-}17}{[\mathrm{CH_2}]_7}\text{-}\overset{18}{\mathrm{CH_3}}\\ \;\Vert\\ \underset{9}{\mathrm{HC}}\text{-}\underset{8\text{-}2}{[\mathrm{CH_2}]_7}\text{-}\underset{1}{\mathrm{CO}}–\end{array}$	P-65.1.7.3.1; P-65.1.7.4.1
octadecyl* = octadecan-1-yl	$\mathrm{CH_3\text{-}[CH_2]_{17}}$–	P-29.3.2.1; P-29.3.2.2
octanoyl* = 1-oxooctyl	$\mathrm{CH_3\text{-}[CH_2]_6\text{-}CO}$–	P-65.1.7.4.1
octan-1-yl = octyl*	$\mathrm{CH_3\text{-}[CH_2]_6\text{-}CH_2}$–	P-29.3.2.1; P-29.3.2.2
octan-1-ylidene = octylidene*	$\mathrm{CH_3\text{-}[CH_2]_6\text{-}CH{=}}$	P-29.3.2.1; P-29.3.2.2
octanylidyne = octylidyne*	$\mathrm{CH_3\text{-}[CH_2]_6\text{-}C{\equiv}}$	P-29.3.2.1; P-29.3.2.2
octyl* = octan-1-yl	$\mathrm{CH_3\text{-}[CH_2]_6\text{-}CH_2}$–	P-29.3.2.1; P-29.3.2.2
octylidene* = octan-1-ylidene	$\mathrm{CH_3\text{-}[CH_2]_6\text{-}CH{=}}$	P-29.3.2.1; P-29.3.2.2
octylidyne* = octanylidyne	$\mathrm{CH_3\text{-}[CH_2]_6\text{-}C{\equiv}}$	P-29.3.2.1; P-29.3.2.2
oleoyl = (9*Z*)-octadec-9-enoyl* = (9*Z*)-1-oxooctadec-9-en-1-yl	 $\begin{array}{l}\overset{10}{\mathrm{HC}}\text{-}\overset{11\text{-}17}{[\mathrm{CH_2}]_7}\text{-}\overset{18}{\mathrm{CH_3}}\\ \;\Vert\\ \underset{9}{\mathrm{HC}}\text{-}\underset{8\text{-}2}{[\mathrm{CH_2}]_7}\text{-}\underset{1}{\mathrm{CO}}–\end{array}$	P-65.1.7.3.1; P-65.1.7.4.1
oxalimidoyl = ethanediimidoyl* = diiminoethanediyl	–C(=NH)-C(=NH)–	P-65.1.7.2.2
oxalo* = carboxycarbonyl (not carboxyformyl; not hydroxy(oxo)acetyl)	HO-CO-CO–	P-65.1.2.2.3; P-65.1.7.2.1

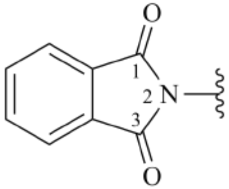
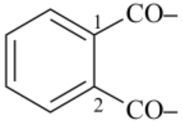
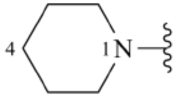
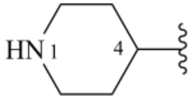
oxaloamino* = (carboxycarbonyl)amino	HOOC-CO-NH–	P-65.1.7.2.4
2-oxaloethyl: see 3-carboxy-3-oxopropyl*		
oxalooxy* = (carboxycarbonyl)oxy [not (carboxyformyl)oxy]	HO-CO-CO-O–	P-65.1.7.2.4
oxalosulfanyl* = (carboxycarbonyl)sulfanyl = (carboxycarbonyl)thio [not (carboxyformyl)sulfanyl; not (carboxyfomyl)thio]	HOOC-CO-S–	P-65.1.7.2.4
oxalyl* = ethanedioyl = dioxoethanediyl	–CO-CO–	P-65.1.7.2.1
oxalylbis(azanediyl)* = ethanedioylbis(azanediyl)	–HN-CO-CO-NH–	P-66.1.1.4.5.2
oxalylbis(azanetriyl) = oxalyldinitrilo* = ethanedioyldinitrilo = ethanedioylbis(azanetriyl)	>N-CO-CO-N<	P-66.1.1.4.5.2
oxalylbis(azanylylidene)* = ethanedioylbis(azanylylidene)	=N-CO-CO-N=	P-66.1.1.4.5.2
oxalyldinitrilo* = oxalylbis(azanetriyl) = ethanedioyldinitrilo = ethanedioylbis(azanetriyl)	>N-CO-CO-N<	P-66.1.1.4.5.2
oxamoyl* = aminooxalyl = amino(oxo)acetyl (not carbamoylformyl; not carbamoycarbonyl)	H_2N-CO-CO–	P-66.1.1.4.1.2
oxamoylamino* = amino(oxo)acetamido (not carbamoylformamido)	H_2N-CO-CO-NH–	P-66.1.1.4.5.1
oxamoylazanediyl*	H_2N-CO-CO-N<	P-66.1.1.4.5.2
oxamoylimino* = [amino(oxo)acetyl]imino	H_2N-CO-CO-N=	P-66.1.1.4.5.1
oxidanyl: see hydroxy*		
oxido*	$^{-}$O–	P-72.6.2
oxo* (not keto)	O=	P-64.5.1
oxoacetyl*	OCH-CO–	P-65.1.6.3; P-65.1.7.2.4
oxoarsanyl* (not arsenoso)	O=As–	P-61.6
oxo-λ^5-azanyl*	H_2N(O)–	P-62.5
(oxo-λ^5-azanylidyne)methyl* (not isofulminato)	ON≡C–	P-61.10; P-66.5.4.2
1-oxobutyl = butanoyl* = butyryl	CH_3-CH_2-CH_2-CO–	P-65.1.7.3.1; P-65.1.7.4.1
1-oxodecyl = decanoyl*	CH_3-[CH_2]$_8$-CO–	P-65.1.7.4.1
1-oxododecyl = dodecanoyl*	CH_3-[CH_2]$_{10}$-CO–	P-65.1.7.4.1
1-oxoethyl = acetyl* = ethanoyl	CH_3-CO–	P-65.1.7.2.1
1-oxoheptyl = heptanoyl*	CH_3-[CH_2]$_5$-CO–	P-65.1.7.4.1
1-oxohexadecyl = hexadecanoyl* = palmitoyl	CH_3-[CH_2]$_{14}$-CO–	P-65.1.7.3.1; P-65.1.7.4.1
1-oxohexyl = hexanoyl*	CH_3-[CH_2]$_4$-CO–	P-65.1.7.4.1
oxolan-3-yl-4-ylidene*		P-29.3.3
oxomethyl = formyl* = methanoyl	HCO–	P-65.1.7.2.1; P-66.6.1.3
oxomethylidene*	O=C=	P-65.2.1.8
1-oxononyl = nonanoyl*	CH_3-[CH_2]$_7$-CO–	P-65.1.7.4.1

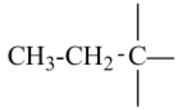
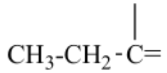
(9*Z*)-1-oxooctadec-9-en-1-yl = (9*Z*)-octadec-9-enoyl* = oleoyl	 $\begin{array}{l} \overset{10}{\mathrm{HC}}\text{-}\overset{11\text{-}17}{[\mathrm{CH_2}]_7}\text{-}\overset{18}{\mathrm{CH_3}} \\ \,\,\| \\ \underset{9}{\mathrm{HC}}\text{-}\underset{8\text{-}2}{[\mathrm{CH_2}]_7}\text{-}\underset{1}{\mathrm{CO}}– \end{array}$	P-65.1.7.3.1; P-65.1.7.4.1
1-oxooctadecyl = octadecanoyl* = stearoyl	CH$_3$-[CH$_2$]$_{16}$-CO–	P-65.1.7.3.1; P-65.1.7.4.1
1-oxooctyl = octanoyl*	CH$_3$-[CH$_2$]$_6$-CO–	P-65.1.7.4.1
1-oxopentyl = pentanoyl*	CH$_3$-CH$_2$-CH$_2$-CH$_2$-CO–	P-65.1.7.4.1
oxo(phenyl)methyl = benzoyl* = benzenecarbonyl = phenylcarbonyl	C$_6$H$_5$-CO–	P-34.2.1.1; P-34.2.2; P-65.1.7.2.1
oxophosphanyl* (not phosphoroso)	O=P–	P-61.6; P-67.1.4.1.1.6
oxo-λ^5-phosphanylidene*	HP(O)=	P-67.1.4.1.1.6
oxo-λ^5-phosphanylidyne*	P(O)≡	P-67.1.4.1.1.6
2-oxopropanoyl* = 1,2-dioxopropyl (not pyruvoyl)	CH$_3$-CO-CO–	P-65.1.1.2.3; P-65.1.7.4.1
1-oxoprop-2-en-1-yl = prop-2-enoyl* = acryloyl	CH$_2$=CH-CO–	P-65.1.7.3.1; P-65.1.7.4.1
1-oxopropyl = propanoyl* = propionyl	CH$_3$-CH$_2$-CO–	P-65.1.7.3.1; P-65.1.7.4.1
2-oxopropyl* = acetonyl	CH$_3$-CO-CH$_2$–	P-64.5.1
2-oxopropylidene* (not acetonylidene)	CH$_3$-CO-CH=	P-64.5
2-oxopropylidyne* (not acetonylidyne)	CH$_3$-CO-C≡	P-64.5
oxo(pyridin-3-yl)methyl = nicotinyl = pyridine-3-carbonyl* = 3-pyridylcarbonyl	3-C$_5$H$_4$N-CO–	P-65.1.7.3.1; P-65.6.3.2.3
oxo(pyridin-4-yl)methyl = isonicotinyl = pyridine-4-carbonyl* = 4-pyridylcarbonyl	4-C$_5$H$_4$N-CO–	P-65.1.7.3.1; P-65.1.7.4.2
oxostibanyl*	O=Sb–	P-67.1.4.1.1.6
1-oxo-4-sulfanylidenebutane-1,4-diyl*	–CO-CH$_2$CH$_2$-CS–	P-65.1.7.5
1-oxotetradecyl = tetradecanoyl*	CH$_3$-[CH$_2$]$_{12}$-CO–	P-65.1.7.4.1
oxy*	–O–	P-15.3.1.2.1.1; P-63.2.2.1.1
oxylcarbonyl* = (ylooxidanyl)formyl	$^{\bullet}$O-CO–	P-71.5
palmitoyl = hexadecanoyl* = 1-oxohexadecyl	CH$_3$-[CH$_2$]$_{14}$-CO–	P-65.1.7.3.1; P-65.1.7.4.1
pentanedioyl* = glutaryl = 1,5-dioxopentane-1,5-diyl	–CO-CH$_2$-CH$_2$-CH$_2$-CO–	P-65.1.7.3.1; P-65.1.7.4.1
pentanoyl* = 1-oxopentyl	CH$_3$-CH$_2$-CH$_2$-CH$_2$-CO–	P-65.1.7.4.1
pentan-1-yl = pentyl*	CH$_3$-CH$_2$-CH$_2$-CH$_2$-CH$_2$–	P-29.3.2.1 ;P-29.3.2.2
pentan-2-yl* = 1-methylbutyl	CH$_3$-CH$_2$-CH$_2$-CH(CH$_3$)–	P-29.3.2.2; P-29.4.1
pentan-1-ylidene = pentylidene*	CH$_3$-CH$_2$-CH$_2$-CH$_2$-CH=	P-29.3.2.1; P-29.3.2.2
pentan-3-ylidene* = 1-ethylpropylidene	(CH$_3$-CH$_2$)$_2$C=	P-29.3.2.2; P-29.4
pentanylidyne = pentylidyne*	CH$_3$-CH$_2$-CH$_2$-CH$_2$-C≡	P-29.3.2.1; P-29.3.2.2
pent-2-enoyl*	CH$_3$-CH$_2$-CH=CH-CO–	P-65.1.7.4.1
pentyl* = pentan-1-yl	CH$_3$-CH$_2$-CH$_2$-CH$_2$-CH$_2$–	P-29.3.2.1; P-29.3.2.2
tert-pentyl: see 2-methylbutan-2-yl*		
pentylidene* = pentan-1-ylidene	CH$_3$-CH$_2$-CH$_2$-CH$_2$-CH=	P-29.3.2.1; P-29.3.2.2
pentylidyne* = pentanylidyne	CH$_3$-CH$_2$-CH$_2$-CH$_2$-C≡	P-29.3.2.1; P-29.3.2.2

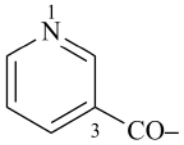
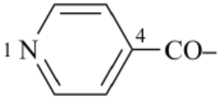
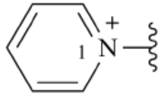
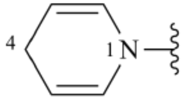
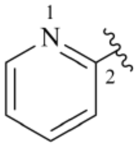
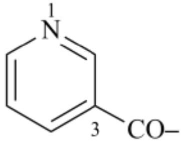
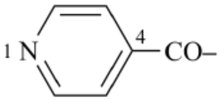
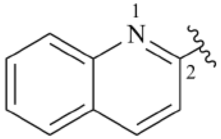
pentyloxy*	CH_3-$[CH_2]_3$-CH_2-O–	P-63.2.2.1.1
perbromyl*	O_3Br–	P-61.3.2.3
perchloryl*	O_3Cl–	P-61.3.2.3
perfluoryl*	O_3F–	P-61.3.2.3
periodyl*	O_3I–	P-61.3.2.3
peroxy* (not dioxy)	–OO–	P-63.3.1
peroxycarboxy: see carbonoperoxoyl*		
peroxyphosphoryl = phosphoroperoxoyl* = (hydroperoxy)phosphoryl	(HOO)-P(O)<	P-67.1.4.1.1.4
phenanthren-9-yl* = 9-phenanthryl (also 1-, 2-, 3-, and 4-isomers)		P-29.3.4.1; P-29.6.2.3; P-57.1.5.3
9-phenanthryl = phenanthren-9-yl* (also 1-, 2-, 3-, and 4-isomers)	9-$C_{14}H_9$–	P-29.3.4.1; P-29.6.2.3; P-57.1.5.3
phenethyl: see 2-phenylethyl		
o-phenetidino: see 2-ethoxyanilino* (also *m* = 3 and *p* = 4 isomers)		
phenoxy* (not phenyloxy)	C_6H_5-O–	P-63.2.2.2
phenyl*	C_6H_5–	P-29.6.1
phenylamino = anilino*	C_6H_5-NH–	P-62.2.1.1.1
(phenylamino)sulfonyl = phenylsulfamoyl* = anilinosulfonyl	C_6H_5-NH-SO_2–	P-66.1.1.4.2
phenylazo = phenyldiazenyl*	C_6H_5-N=N–	P-68.3.1.3.2.2
phenylcarbonyl = benzoyl* = benzenecarbonyl = oxo(phenyl)methyl	C_6H_5-CO–	P-34.2.1.1; P-34.2.2; P-65.1.7.2.1
(phenylcarbonyl)oxy = benzoyloxy*	C_6H_5-CO-O–	P-65.6.3.2.3
phenyl(chlorophosphonoyl) = phenylphosphonochloridoyl*	(C_6H_5)ClP(O)–	P-67.1.4.1.1.4
phenyldiazenyl* = phenylazo	C_6H_5–N=N–	P-68.3.1.3.2.2
1,2-phenylene* (not benzene-1,2-diyl) (also 1,3- and 1,4-isomers)		P-29.6.1
1,4-phenylenebis(iminomethylene) = benzene-1,4-dicarboximidoyl* = terephthalimidoyl = 1,4-phenylenedicarbonimidoyl		P-65.1.7.3.2
1,2-phenylenebis(oxomethylene) = benzene-1,2-dicarbonyl* = phthaloyl = 1,2-phenylenedicarbonyl	1,2-C_6H_4(CO–)$_2$	P-65.1.7.3.1; P-65.1.7.4.2
1,3-phenylenebis(oxomethylene) = benzene-1,3-dicarbonyl* = isophthaloyl = 1,3-phenylenedicarbonyl	1,3-C_6H_4(CO–)$_2$	P-65.1.7.3.1; P-65.1.7.4.2
1,4-phenylenebis(oxomethylene) = benzene-1,4-dicarbonyl* = terephthaloyl	1,4-C_6H_4(CO–)$_2$	P-65.1.7.3.1; P-65.1.7.4.2

= 1,4-phenylenedicarbonyl		
1,2-phenylenebis(sulfanylidenemethylene) = benzene-1,2-dicarbothioyl* = 1,2-phenylenebis(thioxomethylene) (not dithiophthaloyl)	1,2-$C_6H_4(CS–)_2$	P-65.1.7.3.1; P-65.1.7.4.3
1,2-phenylenebis(thioxomethylene) = benzene-1,2-dicarbothioyl* = 1,2-phenylenebis(sulfanylidenemethylene) (not dithiophthaloyl)	1,2-$C_6H_4(CS–)_2$	P-65.1.7.3.1; P-65.1.7.4.3
1,4-phenylenedicarbonimidoyl = benzene-1,4-dicarboximidoyl* = terephthalimidoyl = 1,4-phenylenebis(iminomethylene)	1,4-$C_6H_4(C{=}NH)_2–$	P-65.1.7.3.2
1,2-phenylenedicarbonyl = benzene-1,2-dicarbonyl* = phthaloyl = 1,2-phenylenebis(oxomethylene)		P-65.1.7.3.1; P-65.1.7.4.2
1,3-phenylenedicarbonyl = benzene-1,3-dicarbonyl* = isophthaloyl = 1,3-phenylenebis(oxomethylene)		P-65.1.7.3.1; P-65.1.7.4.2
1,4-phenylenedicarbonyl = benzene-1,4-dicarbonyl* = terephthaloyl = 1,4-phenylenebis(oxomethylene)		P-65.1.7.3.1; P-65.1.7.4.2
2-phenylethenyl* = 2-phenylvinyl = styryl	C_6H_5-CH=CH–	P-32.3
2-phenylethyl* (not phenethyl)	C_6H_5-CH_2-CH_2–	P-29.6.3
phenylmethoxy = benzyloxy*	C_6H_5-CH_2-O–	P-63.2.2.1.1
phenylmethyl = benzyl*	C_6H_5-CH_2–	P-29.6.1; P-29.6.2.1
phenylmethylidene = benzylidene* (not benzal)	C_6H_5-CH=	P-29.6.1; P-29.6.2.1
phenylmethylidyne = benzylidyne*	C_6H_5-C≡	P-29.6.1; P-29.6.2.1
phenyloxy: see phenoxy*		
4-phenylphenyl: see [1,1′-biphenyl]-4-yl		
phenylphosphonochloridoyl* = phenyl(chlorophosphonoyl)	(C_6H_5)ClP(O)–	P-67.1.4.1.1.4
3-phenylprop-2-enoyl* = cinnamoyl	C_6H_5-CH=CH-CO–	P-65.1.7.3.1
phenylselanyl* = phenylseleno	C_6H_5-Se–	P-63.2.2.1.2; P-63.2.5
(phenylselanyl)oxy*	C_6H_5-Se-O–	P-63.3.2
phenylseleno = phenylselanyl*	C_6H_5-Se–	P-63.2.2.1.2; P-63.2.5
phenylselenonyl = benzeneselenonyl*	C_6H_5-SeO_2–	P-65.3.2.2.2
phenylsulfamoyl* = (phenylamino)sulfonyl = anilinosulfonyl	C_6H_5-NH-SO_2–	P-66.1.1.4.2
phenylsulfanyl* = phenylthio	C_6H_5-S–	P-63.2.2.1.2; P-63.2.5
phenyl(sulfanylidene)methyl = benzenecarbothioyl* = thiobenzoyl = phenyl(thioxo)methyl	C_6H_5-CS–	P-65.1.7.2.3
(phenylsulfanyl)oxy*	C_6H_5-S-O–	P-63.3.2
phenylsulfinoselenoyl = benzenesulfinoselenoyl*	C_6H_5-S(Se)–	P-65.3.2.2.2
phenylsulfinyl = benzenesulfinyl*	C_6H_5-S(O)–	P-63.6; P-65.3.2.2.2
(phenylsulfinyl)amino = benzenesulfinamido* = (benzenesulfinyl)amino	C_6H_5-S(O)-NH–	P-66.1.1.4.3

phenylsulfonyl = benzenesulfonyl*	C_6H_5-SO_2–	P-63.6; P-65.3.2.2.2
(phenylsulfonyl)amino = benzenesulfonamido* = (benzenesulfonyl)amino	C_6H_5-SO_2-NH–	P-66.1.1.4.3
phenyltellanyl* = phenyltelluro	C_6H_5-Te–	P-63.2.2.1.2; P-63.2.5
(phenyltellanyl)oxy*	C_6H_5-Te-O–	P-63.3.2
phenyltelluro = phenyltellanyl*	C_6H_5-Te–	P-63.2.2.1.2; P-63.2.5
phenylthio = phenylsulfanyl*	C_6H_5-S–	P-63.2.2.1.2; P-63.2.5
phenyl(thioxo)methyl = benzenecarbothioyl* = thiobenzoyl = phenyl(sulfanylidene)methyl	C_6H_5-CS–	P-65.1.7.2.3
2-phenylvinyl = 2-phenylethenyl* = styryl	C_6H_5-CH=CH–	P-32.3
phosphanediyl* (not phosphinediyl)	HP<	P-68.3.2.3.2.2
phosphanetriyl* (not phosphinetriyl)	–P<	P-68.3.2.3.2.2
phosphaniumyl* = phosphonio = phosphoniumyl	H_3P^+–	P-73.6; P-74.1.3
phosphanyl* = phosphino	H_2P–	P-29.3.1; P-68.3.2.3.2.2
λ^5-phosphanyl* = phosphoranyl	H_4P–	P-68.3.2.3.2.2
phosphanylidene*	HP=	P-29.3.1; P-68.3.2.3.2.2
phosphanylylidene*	–P=	P-68.3.2.3.2.2
phosphinane-3,5-diyl*		P-29.3.3
phosphinediyl: see phosphanediyl*		
phosphinetriyl: see phosphanetriyl*		
phosphinimidoyl* = imidophosphinoyl = dihydrophosphorimidoyl	H_2P(=NH)–	P-67.1.4.1.1.4; P-67.1.4.1.2
phosphino = phosphanyl*	H_2P–	P-29.3.1; P-68.3.2.3.2.2
phosphinothioyl* = thiophosphinoyl = dihydrophosphorothioyl	H_2P(S)–	P-67.1.4.1.1.4; P-67.1.4.1.2
phosphinoyl* = dihydrophosphoryl (not phosphinyl)	H_2P(O)–	P-67.1.4.1.1.2; P-67.1.4.1.2
phosphinyl: see phosphinoyl*		
phospho: see dioxo-λ^5-phosphanyl*		
phosphonato*	$(O^-)_2P(O)$–	P-72.6.1
phosphonio = phosphaniumyl* = phosphoniumyl	H_3P^+–	P-73.6; P-74.1.3
phosphoniumyl = phosphaniumyl* = phosphonio	H_3P^+–	P-73.6; P-74.1.3
phosphono*	$(HO)_2P(O)$–	P-67.1.4.1.1.1
phosphonooxy*	$(HO)_2P(O)$-O–	P-67.1.4.1.3
phosphonothioyl* = hydro(thiophosphoryl)	HP(S)<	P-67.1.4.1.2
phosphonoyl* = hydrophosphoryl	HP(O)<	P-67.1.4.1.1.2; P-67.1.4.1.2
phosphoramidochloridoyl* = amidochlorophosphoryl (not chloroamidophosphoryl)	$(H_2N)ClP(O)$–	P-67.1.4.1.1.4; P-67.1.5.2
phosphoranyl = λ^5-phosphanyl*	H_4P–	P-68.3.2.3.2.2
phosphorocyanidoisocyanatidothioyl* = cyano(isocyanato)phosphorothioyl	(OCN)(NC)P(S)–	P-67.1.4.1.1.4

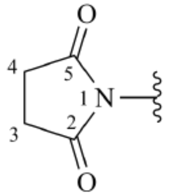
= cyano(isocyanato)thiophosphoryl		
phosphorodichloridoyl* = dichlorophosphoryl	$Cl_2P(O)$–	P-67.1.4.1.1.4
phosphorohydrazidimidoyl* = hydrazidimidophosphoryl	$(H_2N\text{-}NH)\text{-}P(=NH)<$	P-67.1.4.1.1.4
phosphoronitridoyl* = nitridophosphoryl	N≡P<	P-67.1.4.1.1.4
phosphoroperoxoyl* = peroxyphosphoryl = (hydroperoxy)phosphoryl	(HOO)-P(O)<	P-67.1.4.1.1.4
phosphoroso: see oxophosphanyl*		
phosphoro(thioperoxoyl)* = (thioperoxy)phosphoryl = (thiohydroperoxy)phosphoryl	(HSO)-P(O)< or (HOS)-P(O)<	P-67.1.4.1.1.4
phosphorothioyl* = thiophosphoryl	–P(S)<	P-67.1.4.1.1.4
phosphoryl*	–P(O)<	P-67.1.4.1.1.2
phthalimido = 1,3-dioxo-1,3-dihydro-2*H*-isoindol-2-yl*		P-66.2.2
phthaloyl = benzene-1,2-dicarbonyl* = 1,2-phenylenedicarbonyl = 1,2-phenylenebis(oxomethylene)		P-65.1.7.3.1; P-65.1.7.4.2
piperidino = piperidin-1-yl* = 1-piperidyl	$C_5H_{10}N$–	P-29.6.2.3; P-57.1.5.3
piperidin-1-yl* = 1-piperidyl = piperidino		P-29.6.2.3; P-57.1.5.3
piperidin-4-yl* = 4-piperidyl (also 1-, 2-, and 3-isomers) 4-piperidyl = piperidin-4-yl*		P-29.6.2.3; P-57.1.5.3
1-piperidyl = piperidin-1-yl* = piperidino	$C_5H_{10}N$–	P-29.6.2.3; P-57.1.5.3
plumbanediyl* (not plumbylene)	$H_2Pb<$	P-68.2.2
plumbanediylidene*	=Pb=	P-68.2.2
plumbanetetrayl*	>Pb<	P-68.2.2
plumbanetriyl*	–PbH<	P-68.2.2
plumbanyl = plumbyl*	H_3Pb–	P-29.3.1; P-68.2.2
plumbanylidene = plumbylidene*	$H_2Pb=$	P-29.3.1; P-68.2.2
plumbanylidyne = plumbylidyne*	HPb≡	P-29.3.1; P-68.2.2
plumbanylylidene*	–PbH=	P-68.2.2
plumbyl* = plumbanyl	H_3Pb–	P-29.3.1; P-68.2.2
plumbylene: see plumbanediyl*		
plumbylidene* = plumbanylidene	$H_2Pb=$	P-29.3.1; P-68.2.2

plumbylidyne* = plumbanylidyne	HPb≡	P-29.3.1; P-68.2.2
propanamido* = propanoylamino = propionamido = propionylamino	CH_3-CH_2-CO-NH–	P-66.1.1.4.3
propanediimidoyl* = malonimidoyl = 1,3-diiminopropane-1,3-diyl	–C(=HN)-CH_2-C(=NH)–	P-65.1.7.4.1
propanedioyl* = malonyl = 1,3-dioxopropane-1,3-diyl	–CO-CH_2-CO–	P-65.1.7.3.1; P-65.1.7.4.1
propane-1,3-diyl* (not trimethylene)	–CH_2-CH_2-CH_2–	P-29.3.2.2
propane-1,2-diyl* = 1-methylethane-1,2-diyl (not propylene)	–CH_2-CH(CH_3)–	P-29.3.2.2
propane-1,1,1-triyl*	 $CH_3\text{-}CH_2\text{-}\overset{\vert}{\underset{\vert}{C}}\text{—}$	P-29.3.2.2
propanethioyl* = thiopropionyl = 1-sulfanylidenepropyl = 1-thioxopropyl	CH_3-CH_2-CS–	P-65.1.7.4.1
propanimidoyl* = propionimidoyl = 1-iminopropyl	CH_3-CH_2-C(=NH)–	P-65.1.7.3.2; P-65.1.7.4.1
propanoyl* = propionyl = 1-oxopropyl	CH_3-CH_2-CO–	P-65.1.7.3.1; P-65.1.7.4.1
propanoylamino = propanamido* = propionamido = propionylamino	CH_3-CH_2-CO-NH–	P-66.1.1.4.3
propanoyloxy* = propionyloxy	CH_3-CH_2-CO-O–	P-65.6.3.2.3
propan-1-yl = propyl*	CH_3-CH_2-CH_2–	P-29.3.2.1; P-29.3.2.2
propan-2-yl* = isopropyl = 1-methylethyl	$(CH_3)_2$CH–	P-29.3.2.2; P-29.4.1; P-29.6.2.2
propan-1-ylidene = propylidene*	CH_3-CH_2-CH=	P-29.3.2.1; P-29.3.2.2
propan-2-ylidene* = 1-methylethylidene = isopropylidene	$(CH_3)_2$C=	P-29.3.2.2; P-29.4.1; P-29.6.2.2
propanylidyne = propylidyne*	CH_3-CH_2-C≡	P-29.3.2.1; P-29.3.2.2
(propan-2-yl)oxy* = isopropoxy = 1-methylethoxy	$(CH_3)_2$CH-O–	P-63.2.2.2
propan-1-yl-1-ylidene*	 $CH_3\text{-}CH_2\text{-}\overset{\vert}{C}\text{=}$	P-29.3.2.2
prop-2-enehydrazonoyl* = acrylohydrazonoyl = 1-hydrazinylideneprop-2-en-1-yl	CH_2=CH-C(=NNH_2)–	P-65.1.7.3.2
prop-2-eneselenoyl* = selenoacryloyl = 1-selanylideneprop-2-en-1-yl	CH_2=CH-C(Se)–	P-65.1.7.3.3
prop-2-enoyl* = acryloyl = 1-oxoprop-2-en-1-yl	CH_2=CH-CO–	P-65.1.7.3.1; P-65.1.7.4.1
prop-1-en-1-yl*	CH_3-CH=CH–	P-32.1.1
prop-1-en-2-yl* = 1-methylethen-1-yl = isopropenyl	CH_2=C(CH_3)–	P-32.1.1; P-32.3
prop-2-en-1-yl* = allyl	CH_2=CH-CH_2–	P-32.1.1; P-32.3
prop-2-en-1-ylidene* = allylidene	CH_2=CH-CH=	P-32.1.1; P-32.3
prop-2-en-1-ylidyne* = allylidyne	CH_2=CH-C≡	P-32.1.1; P-32.3
propionamido = propanamido* = propionylamino = propanoylamino	CH_3-CH_2-CO-NH–	P-66.1.1.4.3
propionimidoyl = propanimidoyl* = 1-iminopropyl	CH_3-CH_2-C(=NH)–	P-65.1.7.3.2; P-65.1.7.4.1
propionyl = propanoyl* = 1-oxopropyl	CH_3-CH_2-CO–	P-65.1.7.3.1; P-65.1.7.4.1
propionylamino = propanamido* = propanoylamino = propionamido	CH_3-CH_2-CO-NH–	P-66.1.1.4.3
propionyloxy = propanoyloxy*	CH_3-CH_2-CO-O–	P-65.6.3.2.3
propoxy* (not propyloxy)	CH_3-CH_2-CH_2-O–	P-63.2.2.2

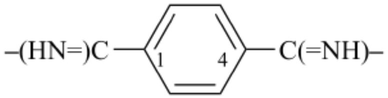
propyl* = propan-1-yl	CH_3-CH_2-CH_2–	P-29.3.2.1; P-29.3.2.2
propylene: see propane-1,2-diyl*		
propylidene* = propan-1-ylidene	CH_3-CH_2-CH=	P-29.3.2.1; P-29.3.2.2
propylidyne* = propanylidyne	CH_3-CH_2-C≡	P-29.3.2.1; P-29-3.2.2
propyloxy: see propoxy*		
pyridine-3-carbonyl* = nicotinoyl = 3-pyridylcarbonyl = oxo(pyridin-3-yl)methyl		P-65.1.7.3.1; P-65.6.3.2.3
pyridine-4-carbonyl* = 4-pyridylcarbonyl = isonicotinoyl = oxo(pyridin-4-yl)methyl		P-65.1.7.3.1; P-65.1.7.4.2
pyridinio = pyridin-1-ium-1-yl* pyridin-1-ium-1-yl* = pyridinio		P-73.6
pyridin-1(4*H*)-yl* (also 1(2*H*)-isomer)		P-29.3.4.1; P-29.6.2.3
pyridin-2-yl* = 2-pyridyl (also 3- and 4- isomers) 2-pyridyl = pyridin-2-yl* (also 3- and 4- isomers)		P-29.3.4.1; P-29.6.2.3; P-57.1.5.3
3-pyridylcarbonyl = pyridine-3-carbonyl* = nicotinoyl = oxo(pyridin-3-yl)methyl		P-65.1.7.3.1; P-65.6.3.2.3
4-pyridylcarbonyl = pyridine-4-carbonyl * = isonicotinoyl = oxo(pyridin-4-yl)methyl		P-65.1.7.3.1; P-65.1.7.4.2
pyruvoyl: see 2-oxopropanoyl*		
quinolin-2-yl* = 2-quinolyl (and 3-, 4-, 5-, 6-, 7-, and 8-isomers) 2-quinolyl = quinolin-2-yl*		P-29.6.2.3; P-57.1.5.3
selanediyl* (not seleno)	–Se–	P-63.2.5
selaniumyl* = selenonio = selenoniumyl	H_2Se^+–	P-73.6
selano* = episeleno (ring forming)	–Se–	P-25.4.2.1.4; P-63.5
selanyl* (not hydroseleno)	HSe–	P-63.1.5

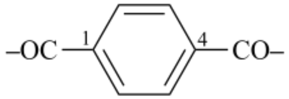
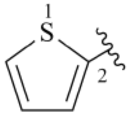
selanylidene* = selenoxo	Se=	P-29.3.1; P-64.6.1
1-selanylideneethyl = ethaneselenoyl* = selenoacetyl	CH_3-C(Se)–	P-65.1.7.2.3
selanylidenemethyl = methaneselenoyl* = selenoformyl	HC(Se)–	P-65.1.7.2.3; P-66.6.3
1-selanylideneprop-2-en-1-yl = prop-2-eneselenoyl* = selenoacryloyl	CH_2=CH-C(Se)–	P-65.1.7.3.3
selanylphosphonoyl*	HP(O)(SeH)–	P-67.1.4.1.1.5
seleneno: see hydroxyselanyl*		
selenino* (unmodified)	HO-Se(O)–	P-65.3.0; P-65.3.2.1
seleninyl*	O=Se<	P-65.3.2.3
seleno: see selanediyl*		
selenoacetyl = ethaneselenoyl* = 1-selanylideneethyl	CH_3-C(Se)–	P-65.1.7.2.3
selenoacryloyl = prop-2-eneselenoyl* = 1-selanylideneprop-2-en-1-yl	CH_2=CH-C(Se)–	P-65.1.7.3.3
selenocyanato* = carbononitridoylselanyl	NC-Se–	P-65.2.2
selenoformyl = methaneselenoyl* = selanylidenemethyl	HC(Se)–	P-65.1.7.2.3; P-66.6.3
OSe-selenohydroperoxy = hydroxyselanyl* (not seleneno)	HO-Se–	P-63.4.2.2
(*OSe*-selenohydroperoxy)methyl = (hydroxyselanyl)methyl*	(HO-Se)-CH_2–	P-63.4.2.2
selenonimidothioyl*	Se(=NH)(=S)<	P-65.3.2.3
selenonio = selaniumyl* = selenoniumyl	H_2Se^+–	P-73.6
selenoniumyl = selaniumyl* = selenonio	H_2Se^+–	P-73.6
selenono* (unmodified)	HO-SeO_2–	P-65.3.0; P-65.3.2.1
selenonohydrazonoyl*	Se(O)(=N-NH_2)<	P-65.3.2.3
selenonyl*	–SeO_2–	P-65.3.2.3
selenoxo = selanylidene*	Se=	P-29.3.1; P-64.6.1
semicarbazido = 2-carbamoylhydrazin-1-yl* = 2-(aminocarbonyl)hydrazine-1-yl	H_2N-CO-NH-NH–	P-68.3.1.2.4
semicarbazono = carbamoylhydrazinylidene*	H_2N-CO-NH-N=	P-68.3.1.2.5
silanediyl* (not silylene)	H_2Si<	P-29.3.1; P-68.2.2
silanediyldi(ethane-2,1-diyl)* = silanediyldiethylene	–CH_2-CH_2-SiH_2-CH_2-CH_2–	P-29.4.2
silanediyldiethylene = silanediyldi(ethane-2,1-diyl)*	–CH_2-CH_2-SiH_2-CH_2-CH_2–	P-29.4.2
silanediylidene*	=Si=	P-68.2.2
silanetetrayl*	>Si<	P-68.2.2
silanetriyl*	–SiH<	P-68.2.2
silanyl = silyl*	H_3Si–	P-29.3.1; P-68.2.2
silanylidene = silylidene*	H_2Si=	P-29.3.1; P-68.2.2
silanylidyne = silylidyne*	HSi≡	P-29.3.1; P-68.2.2
silanylylidene*	–SiH=	P-68.2.2
siloxy: see silyloxy		
silyl* = silanyl	H_3Si–	P-29.3.1; P-68.2.2

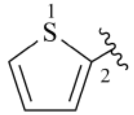
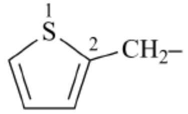
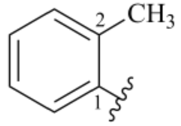
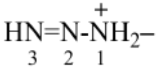
(silylamino)silyl* (not disilazan-1-yl)	$HSi\text{-}NH\text{-}SiH_2–$	P-29.3.2.2
silylene: see silanediyl*		
silylidene* = silanylidene	$H_2Si=$	P-29.3.1; P-68.2.2
silylidyne* = silanylidyne	$HSi≡$	P-29.3.1; P-68.2.2
silyloxy* (not siloxy)	$H_3Si\text{-}O–$	P-63.2.2.1.1
3-silyltetrasilan-1-yl*	$\overset{4}{Si}H_3\text{-}\overset{3}{Si}H(SiH_3)\text{-}\overset{2}{Si}H_2\text{-}\overset{1}{Si}H_2–$	P-29.4.1
stannanediyl* (not stannylene)	$H_2Sn<$	P-68.2.2
stannanediylidene*	$=Sn=$	P-68.2.2
stannanetetrayl*	$>Sn<$	P-68.2.2
stannanetriyl*	$–SnH<$	P-68.2.2
stannanyl = stannyl*	$H_3Sn–$	P-29.3.1; P-68.2.2
stannanylidene = stannylidene*	$H_2Sn=$	P-29.3.1; P-68.2.2
stannanylidyne = stannylidyne*	$HSn≡$	P-29.3.1; P-68.2.2
stannanylylidene*	$–SnH=$	P-68.2.2
stannyl* = stannanyl	$H_3Sn–$	P-29.3.1; P-68.2.2
stannylene: see stannanediyl		
stannylidene* = stannanylidene	$H_2Sn=$	P-29.3.1; P-68.2.2
stannylidyne* = stannanylidyne	$HSn≡$	P-29.3.1; P-68.2.2
stearoyl = octadecanoyl* = 1-oxooctadecyl	$CH_3\text{-}[CH_2]_{16}\text{-}CO–$	P-65.1.7.3.1; P-65.1.7.4.1
stibanediyl* (not stibinediyl)	$HSb<$	P-56.4; P-68.3.2.3.2.2
stibanetriyl* (not stibinetriyl)	$–Sb<$	P-68.3.2.3.2.2
stibaniumyl* = stibonio = stiboniumyl	$H_3Sb^+–$	P-73.6
stibanyl* = stibino	$H_2Sb–$	P-29.3.1; P-68.3.2.3.2.2
λ^5-stibanyl* = stiboranyl	$H_4Sb–$	P-68.3.2.3.2.2
stibanylidene* (not stibinylidene)	$HSb=$	P-29.3.1; P-56.4; P-68.3.2.3.2.2
stibanylylidene*	$–Sb=$	P-68.3.2.3.2.2
stibinediyl: see stibanediyl*		
stibinetriyl: see stibanetriyl*		
stibinimidoyl* = imidostibinoyl = dihydrostiborimidoyl	$H_2Sb(=NH)–$	P-67.1.4.1.1.2; P-67.1.4.1.2
stibino = stibanyl*	$H_2Sb–$	P-29.3.1; P-68.3.2.3.2.2
stibinothioyl* = dihydrostiborothioyl	$H_2Sb(S)–$	P-67.1.4.1.1.2; P-67.1.4.1.2
stibinoyl* = dihydrostiboryl	$H_2Sb(O)–$	P-67.1.4.1.1.2; P-67.1.4.1.2
stibinylidene: see stibanylidene*		
stibonato*	$(^{-}O)_2Sb(O)–$	P-72.6.1
stibonio = stibaniumyl* = stiboniumyl	$H_3Sb^+–$	P-73.6
stiboniumyl = stibaniumyl* = stibonio	$H_3Sb^+–$	P-73.6

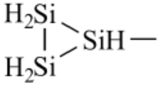
stibono*	(HO)$_2$Sb(O)–	P-67.1.4.1.1.1
stibonoyl* = hydrostiboryl	HSb(O)<	P-67.1.4.1.1.2; P-67.1.4.1.2
stiboranyl = λ^5-stibanyl*	H$_4$Sb–	P-68.3.2.3.2.2
stiborodiamidothioyl*	(H$_2$N)$_2$Sb(S)–	P-67.1.4.1.1.4
stiborohydrazonoyl* = hydrazonostiboryl	Sb(=NNH$_2$)<	P-67.1.4.1.1.4
stiboronitridoyl* = nitridostiboryl	N≡Sb<	P-67.1.4.1.1.4
stiboryl* (not antimonyl)	–Sb(O)<	P-67.1.4.1.1.2
styryl = 2-phenylethenyl* = 2-phenylvinyl	C$_6$H$_5$-CH=CH–	P-32.3
succinimido = 2,5-dioxopyrrolidin-1-yl*		P-66.2.2
succinimidoyl = butanediimidoyl* = 1,4-diiminobutane-1,4-diyl	–C(=NH)-CH$_2$-CH$_2$-C(=NH)–	P-65.1.7.3.2
succinyl = butanedioyl* = 1,4-dioxobutane-1,4-diyl	–CO-CH$_2$-CH$_2$-CO–	P-65.1.7.3.1; P-65.1.7.4.1
sulfamoyl* = aminosulfonyl = sulfuramidoyl	H$_2$N-SO$_2$–	P-65.3.2.3; P-66.1.1.4.2
sulfamoyloxy* = sulfuramidoyloxy	H$_2$N-SO$_2$-O–	P-67.1.4.4.2
sulfanediyl* (not thio; not sulfenyl)	–S–	P-63.2.5
sulfanediylbis(methylene)* (not sulfanediyldimethylene; not thiodimethylene)	–CH$_2$-S-CH$_2$–	P-63.2.2.1.3
sulfanediyldimethylene: see sulfanediylbis(methylene)*		
sulfaniumyl* = sulfoniumyl = sulfonio	H$_2$S$^+$–	P-73.6
sulfano* = epithio (ring forming)	–S–	P-25.4.2.1.4; P-63.5
sulfanyl* (not mercapto)	HS–	P-29.3.1; P-63.1.5
sulfanylbis(sulfanylidene)ethyl = sulfanyl(sulfanylidene)ethanethioyl* = trithiooxalo	HS-CS-CS–	P-65.1.7.2.4; P-65.1.7.3.3
sulfanylboranyl*	HS-BH–	P-67.1.4.2
(*C*-sulfanylcarbonimidoyl)amino* = [imino(sulfanyl)methyl]amino	HS-C(=NH)-NH–	P-66.1.6.1.3.3
sulfanylcarbonothioyl = dithiocarboxy*	HS-CS–	P-65.2.1.6
[(sulfanylcarbonothioyl)sulfanyl]carbonothioyl = [(dithiocarboxy)sulfanyl]carbonothioyl* = [sulfanyl(thiocarbonyl)sulfanyl](thiocarbonyl) {not [(dithiocarboxy)sulfanyl]thioformyl}	HS-CS-S-CS–	P-65.2.3.1.5
sulfanylcarbonyl* (not mercaptocarbonyl)	HS-CO–	P-65.2.1.6
(sulfanylcarbonyl)oxy*	HS-CO-O–	P-65.2.1.6
sulfanylidene* = thioxo	S=	P-29.3.1; P-64.6.1
sulfanylideneamino* = thionitroso = thioxoamino	S=N–	P-67.1.4.3.2
(sulfanylideneamino)sulfanyl* = (thionitroso)sulfanyl = (thioxoamino)sulfanyl	S=N-S–	P-67.1.4.3.2
1-sulfanylidenebutyl = butanethioyl* = thiobutyryl = 1-thioxobutyl	CH$_3$-CH$_2$-CH$_2$-CS–	P-65.1.7.4.1
1-sulfanylideneethyl = ethanethioyl* = thioacetyl	CH$_3$-CS–	P-65.1.7.2.3

sulfanylidenemethyl = methanethioyl* = thioformyl	HCS–	P-65.1.7.2.3; P-66.6.3
sulfanylidenemethylidene* = thioxomethylidene	S=C=	P-65.2.1.8
1-sulfanylidenepropyl = propanethioyl* = thiopropionyl = 1-thioxopropyl	CH$_3$-CH$_2$-CS–	P-65.1.7.4.1
sulfanyloxy* = *SO*-thiohydroperoxy (not mercaptooxy)	HS-O–	P-63.4.2.2
[(sulfanyloxy)carbonyl]oxy* = [(*SO*-thiohydroperoxy)carbonyl]oxy	(HSO)-CO-O–	P-65.2.1.7
(sulfanyloxy)phosphoryl* = (*SO*-thiohydroperoxy)phosphoryl	(HSO)-P(O)<	P-67.1.4.1.1.5
sulfanylphosphonothioyl* = sulfanyl(thiophosphonoyl)	HS-HP(S)–	P-67.1.4.1.1.5
sulfanyl(sulfanylidene)ethanethioyl* = sulfanylbis(sulfanylidene)ethyl = trithiooxalo	HS-CS-CS–	P-65.1.7.2.4; P-65-1.7.3.3
(sulfanylsulfinyl)oxy*	HS-S(O)-O–	P-65.3.2.3
sulfanylsulfonodithioyl = trithiosulfo*	HS-S(S)$_2$–	P-65.3.2.1
[sulfanyl(thiocarbonyl)sulfanyl](thiocarbonyl) = [(dithiocarboxy)sulfanyl]carbonothioyl* = [(sulfanylcarbonothioyl)sulfanyl]carbonothioyl {not [(dithiocarboxy)sulfanyl]thioformyl}	HS-CS-S-CS–	P-65.2.3.1.5
sulfanyl(thiophosphonoyl) = sulfanylphosphonothioyl*	HS-HP(S)–	P-67.1.4.1.1.5
sulfeno: see hydroxysulfanyl*		
sulfenyl: see sulfanediyl*		
sulfido*	$^{-}$S–	P-72.6.2
sulfinamoyl: see aminosulfinyl*		
sulfinamoyloxy: see (aminosulfinyl)oxy*		
sulfinimidoyl*	–S(=NH)–	P-65.3.2.3
sulfino* (when unmodified)	HO-S(O)–	P-65.3.0; P-65.3.2.1
sulfinothioyl*	–S(S)–	P-65.3.2.3
sulfinyl* = thionyl	–S(O)–	P-65.3.2.3
sulfinylbis(oxy)* (not sulfinyldioxy)	–O-S(O)-O–	P-65.3.2.3
sulfinyldioxy: see sulfinylbis(oxy)*		
sulfo* (when unmodified)	HO-SO$_2$–	P-65.3.0; P-65.3.2.1
sulfonato*	$^{-}$O-SO$_2$–	P-72.6.1
sulfonimidoyl* = sulfurimidoyl	–S(O)(=NH)–	P-65.3.2.3; P-67.1.4.4.1
sulfonio = sulfaniumyl* = sulfoniumyl	H$_2$S$^+$–	P-73.6
sulfoniumyl = sulfaniumyl* = sulfonio	H$_2$S$^+$–	P-73.6
sulfonodihydrazonoyl* = sulfurodihydrazonoyl	–S(=N-NH$_2$)$_2$–	P-65.3.2.3; P-67.1.4.4.1
sulfonodiimidoyl* = sulfurodiimidoyl	–S(=NH)$_2$–	P-65.3.2.3; P-67.1.4.4.1
sulfonodithioyl* = sulfurodithioyl	–S(=S)$_2$–	P-65.3.2.3; P-67.1.4.4.1
sulfonohydrazonoyl* = sulfurohydrazonoyl	–S(O)(=NNH$_2$)–	P-65.3.2.3; P-67.1.4.4.1
sulfonothioyl* = sulfurothioyl	–S(O)(S)–	P-65.3.2.3; P-67.1.4.4.1
sulfonyl* = sulfuryl	–SO$_2$–	P-65.3.2.3; P-67.1.4.4.1
sulfonylbis(methylene)* (not sulfonyldimethylene)	–CH$_2$-SO$_2$-CH$_2$–	P-65.3.2.3
sulfonylbis(oxy)* (not sulfonyldioxy)	–O-SO$_2$-O–	P-65.3.2.3

sulfonylbis(sulfanediyl)* (not sulfonyldisulfanediyl)	–S-SO$_2$-S–	P-65.3.2.3
sulfonyldimethylene: see sulfonylbis(methylene)*		
sulfonyldioxy: see sulfonylbis(oxy)*		
sulfonyldisulfanediyl: see sulfonylbis(sulfanediyl)*		
sulfooxy*	HO-SO$_2$-O–	P-65.3.2.3; P-67.1.4.4.2
sulfuramidoyl = sulfamoyl* = aminosulfonyl	H$_2$N-SO$_2$–	P-65.3.2.3; P-66.1.1.4.2
sulfuramidoyloxy = sulfamoyloxy*	H$_2$N-SO$_2$-O–	P-67.1.4.4.2
sulfurimidoyl = sulfonimidoyl*	–S(O)(=NH)–	P-65.3.2.3; P-67.1.4.4.1
sulfur(isothiocyanatido)thioyl = isothiocyanatosulfonothioyl*	(SCN)-S(O)(S)–	P-67.1.4.4.1
sulfur(isothiocyanatidoyl) = isothiocyanatosulfonyl*	(SCN)-SO$_2$–	P-67.1.4.4.1
sulfurochloridoyl = chlorosulfonyl*	Cl-SO$_2$–	P-65.3.2.3; P-67.1.4.4.1
sulfurochloridoyloxy = (chlorosulfonyl)oxy*	Cl-SO$_2$-O–	P-65.3.2.3; P-67.1.4.4.2
sulfurocyanidoyl = cyanosulfonyl*	NC-SO$_2$–	P-67.1.4.4.1
sulfurodihydrazonoyl = sulfonodihydrazonoyl*	–S(=NNH$_2$)$_2$–	P-65.3.2.3; P-67.1.4.4.1
sulfurodiimidoyl = sulfonodiimidoyl*	–S(=NH)$_2$–	P-67.1.4.4.1
sulfurodithioyl = sulfonodithioyl*	–S(S)$_2$–	P-65.3.2.3; P-67.1.4.4.1
sulfurohydrazonoyl = sulfonohydrazonoyl*	–S(O)(=NNH$_2$)–	P-65.3.2.3; P-67.1.4.4.1
sulfurothioyl = sulfonothioyl*	–S(O)(S)–	P-65.3.2.3; P-67.1.4.4.1
sulfuryl = sulfonyl*	–SO$_2$–	P-65.3.2.3; P-67.1.4.4.1
tellanediyl* (not telluro)	–Te–	P-63.2.2.1.2; P-63.2.5
tellano* = epitelluro (ring forming)	–Te–	P-25.4.2.1.4; P-63.5
tellanyl* (not hydrotelluro)	HTe–	P-63.1.5
tellanylidene* = telluroxo	Te=	P-29.3.1; P-64.6.1; P-66.6.3
tellanylidenemethyl = methanetelluroyl* = telluroformyl	HC(Te)–	P-65.1.7.2.3; P-66.6.3
tellureno: see hydroxytellanyl*		
tellurino* (unmodified)	HO-Te(O)–	P-65.3.0; P-65.3.2.1
tellurinyl*	–Te(O)–	P-65.3.2.3
telluro: see tellanediyl*		
tellurocyanato* = carbononitridoyltellanyl	NC-Te–	P-65.2.2
telluroformyl = methanetelluroyl* = tellanylidenemethyl	HC(Te)–	P-65.1.7.2.3; P-66.6.3
OTe-tellurohydroperoxy = hydroxytellanyl* (not tellureno)	HO-Te–	P-63.4.2.2
tellurono* (unmodified)	HO-TeO$_2$–	P-63.3.0; P-65.3.2.1
telluronyl*	–TeO$_2$–	P-65.3.2.3
telluroxo = tellanylidene*	Te=	P-29.3.1, P-64.6.1; P-66.6.3
terephthalimidoyl = benzene-1,4-dicarboximidoyl* = 1,4-phenylenebis(iminomethylene) = 1,4-phenylenedicarbonimidoyl		P-65.1.7.3.2

terephthaloyl = benzene-1,4-dicarbonyl* = 1,4-phenylenedicarbonyl = 1,4-phenylenebis(oxomethylene)		P-65.1.7.3.1; P-65.1.7.4.2
tetraazan-1-yl*	H_2N-NH-NH-NH–	P-68.3.1.4.1
tetradecanoyl* = 1-oxotetradecyl	CH_3-[CH_2]$_{12}$-CO–	P-65.1.7.4.1
tetramethylene: see butane-1,4-diyl*		
tetrasulfanediyl* = tetrathio	–S-S-S-S–	P-68.4.1.2
tetrathio = tetrasulfanediyl*	–S-S-S-S–	P-68.4.1.2
thallanyl*	H_2Tl–	P-29.3.1; P-68.1.2
thenyl (2-isomer only): see (thiophen-2-yl)methyl*		
2-thienyl = thiophen-2-yl* (also 3-isomer)		P-29.6.2.3; P-57.1.5.3
thio: see sulfanediyl*		
thioacetamido = ethanethioamido* = (ethanethioy)amino	CH_3-CS-NH–	P-66.1.4.4
thioacetyl = ethanethioyl* = 1-sulfanylideneethyl	CH_3-CS–	P-65.1.7.2.3
thioazonoyl = azonothioyl*	HN(S)<	P-67.1.4.1.1.4
thiobenzamido = benzenecarbothioamido* = (benzenecarbothioyl)amino	C_6H_5-CS-NH–	P-66.1.4.4
thiobenzoyl = benzenecarbothioyl* = phenyl(sulfanylidene)methyl = phenyl(thioxo)methyl	C_6H_5-CS–	P-65.1.7.2.3
thioborono* = hydroxy(sulfanyl)boranyl	(HO)(HS)B–	P-68.1.4.2
thiobutyryl = butanethioyl* = 1-sulfanylidenebutyl = 1-thioxobutyl	CH_3-CH_2-CH_2-CS–	P-65.1.7.4.1
thiocarbamoyl: see carbamothioyl*		
thiocarbonyl = carbonothioyl*	–CS–	P-65.2.1.5
thiocarboxy* (unspecified)	H{S/O}C–	P-65.2.1.6
(thiocarboxy)carbonyl*	H{S/O}C-CO–	P-65.1.7.2.1; P-65.1.7.2.4
thiochlorosyl*	Cl(S)–	P-67.1.4.5
thiocyanato* = carbononitridoylsulfanyl = carbononitridoylthio	NC-S–	P-65.2.2
thiocyanatosulfanyl: see cyanodisulfanyl*		
thiodimethylene: see sulfanediylbis(methylene)*		
thioformamido = methanethioamido* = (methanethioyl)amino	HCS-NH–	P-66.1.4.4
thioformyl = methanethioyl* = sulfanylidenemethyl	HCS–	P-65.1.7.2.3; P-66.6.3
OS-thiohydroperoxy = hydroxysulfanyl* (not hydroxythio, not sulfeno)	HOS–	P-63.4.2.2
SO-thiohydroperoxy = sulfanyloxy* (not mercaptooxy)	HS-O–	P-63.4.2.2
(*OS*-thiohydroperoxy)carbonoselenoyl = (hydroxysulfanyl)carbonoselenoyl*	(HOS)-C(Se)–	P-65.2.1.7
(thiohydroperoxy)carbonyl = carbono(thioperoxoyl)*	(HOS)-CO– or (HSO)-CO–	P-65.1.5.3; P-65.2.1.7
(*OS*-thiohydroperoxy)carbonyl = (hydroxysulfanyl)carbonyl*	(HOS)-CO–	P-65.1.5.3; P-65.2.1.7
[(*SO*-thiohydroperoxy)carbonyl]oxy = [(sulfanyloxy)carbonyl]oxy*	(HSO)-CO-O–	P-65.2.1.7

(*OS*-thiohydroperoxy)phosphorothioyl = (hydroxysulfanyl)phosphorothioyl*	(HOS)-P(S)<	P-67.1.4.1.1.4; P-67.1.4.1.1.5
(thiohydroperoxy)phosphoryl = phosphoro(thioperoxoyl)* = (thioperoxy)phosphoryl	(HSO)-P(O)< or (HOS)-P(O)<	P-67.1.4.1.1.4
(*SO*-thiohydroperoxy)phosphoryl = (sulfanyloxy)phosphoryl*	(HSO)-P(O)<	P-67.1.4.1.1.5
thionitroso = sulfanylideneamino* = thioxoamino	S=N–	P-67.1.4.3.2
(thionitroso)sulfanyl = (sufanylideneamino)sulfanyl* = (thioxoamino)sulfanyl	S=N-S–	P-67.1.4.3.2
thionyl = sulfinyl*	–S(O)–	P-65.3.2.3
2-thiooxalo: see hydroxy(sulfanylidene)acetyl*		
(thioperoxy)phosphoryl = phosphoro(thioperoxoyl)* = (thiohydroperoxy)phosphoryl	(HSO)-P(O)< or (HOS)-P(O)<	P-67.1.4.1.1.4
thiophen-2-yl* = 2-thienyl (also 3- isomer)		P-29.6.2.3; P-57.1.5.3
(thiophen-2-yl)methyl* (not thenyl)		P-29.6.3
thiophosphinoyl = phosphinothioyl* = dihydrophosphorothioyl	H$_2$P(S)–	P-67.1.4.1.1.4; P-67.1.4.1.2
thiophosphono* (unspecified)	(HO)(HS)P(O)– or (HO)$_2$P(S)–	P-67.1.4.1.1.1
thiophosphoryl = phosphorothioyl*	–P(S)<	P-67.1.4.1.1.4
thiopropionyl = propanethioyl* = 1-sulfanylidenepropyl = 1-thioxopropyl	CH$_3$-CH$_2$-CS–	P-65.1.7.4.1
thiosulfeno: see disulfanyl*		
thiosulfino* (unspecified)	H{S/O}S–	P-65.3.2.1
thiosulfo* (unspecified)	HO$_2$S$_2$–	P-65.3.2.1
thioxo = sulfanylidene*	S=	P-29.3.1; P-64.6.1
thioxoamino = thionitroso = sulfanylideneamino*	S=N–	P-67.1.4.3.2
(thioxoamino)sulfanyl = (sulfanylideneamino)sulfanyl* = (thionitroso)sulfanyl	S=N-S–	P-67.1.4.3.2
1-thioxobutyl = butanethioyl* = 1-sulfanylidenebutyl = thiobutyryl	CH$_3$-CH$_2$-CH$_2$-CS–	P-65.1.7.4.1
thioxomethylidene = sulfanylidenemethylidene*	S=C=	P-65.2.1.8
1-thioxopropyl = propanethioyl* = thiopropionyl = 1-sulfanylidenepropyl	CH$_3$-CH$_2$-CS–	P-65.1.7.4.1
o-toluidino: see 2-methylanilino* (also *m*- and *p*-isomers)		
o-tolyl = 2-methylphenyl* (also *m*- = 3- and *p*- = 4-isomers)		P-29.6.2.3; P-57.1.5.3
triazano: see triazan-1-yl*		
triazan-1-yl* (not triazano)	H$_2$N-NH-NH–	P-29.3.2.2; P-68.3.1.4.1
triaz-1-ene-1,3-diyl* (not diazoamino)	–N=N-NH–	P-68.3.1.4.2
triaz-2-en-1-ium-1-yl* = triaz-2-en-1-io triaz-2-en-1-io = triaz-2-en-1-ium-1-yl*	 $\underset{3}{HN}=\underset{2}{N}\text{-}\underset{1}{\overset{+}{N}}H_2\text{–}$	P-73.6

triaz-2-eno: see triaz-2-en-1-yl*		
triaz-2-en-1-yl* (not triaz-2-eno)	HN=N-NH–	P-32.1.1: P-68.3.1.4.1
triboran(5)-1-yl*	H_2B-BH-BH–	P-68.1.2
tricyclo[3.3.1.1^{3,7}]decan-2-yl = adamantan-2-yl* = 2-adamantyl (also 1-isomer)	$C_{10}H_{15}$–	P-29.6.2.3
trihydroxysilyl*	$(HO)_3Si$–	P-67.1.4.2
trimethoxysilyl*	$(CH_3O)_3Si$–	P-67.1.4.2
trimethylene: see propane-1,3-diyl*		
trioxidanediyl* = trioxy	–O-O-O–	P-68.4.1.2
trioxidanyl* = hydrotrioxy	HO-O-O–	P-68.4.1.3
trioxy = trioxidanediyl*	–O-O-O–	P-68.4.1.2
triphenylmethyl* = trityl (unsubstituted)	$(C_6H_5)_3C$–	P-29.6.2.2
triselanediyl*= triseleno	–Se-Se-Se–	P-68.4.1.2
triselanyl* = hydrotriseleno	HSeSeSe–	P-68.4.1.3
triseleno = triselanediyl	–Se-Se-Se–	P-68.4.1.2
trisilan-2-yl*	$(SiH_3)_2SiH$–	P-29.3.2.2
trisilazan-3-yl: see bis(silylamino)silyl*		
trisiliranyl* = cyclotrisilanyl		P-68.2.2
trisulfanediyl* = trithio	–S-S-S–	P-68.4.1.2
trisulfanyl* = hydrotrithio	HS-S-S–	P-68.4.1.3
tritellanediyl*= tritelluro	–Te-Te-Te–	P-68.4.1.2
tritellanyl* = hydrotritelluro	HTe-Te-Te–	P-68.4.1.3
tritelluro = tritellanediyl*	–Te-Te-Te–	P-68.4.1.2
trithio = trisulfanediyl*	–S-S-S–	P-68.4.1.2
trithiooxalo = sulfanyl(sulfanylidene)ethanethioyl* = sulfanylbis(sulfanylidene)ethyl	HS-CS-CS–	P-65.1.7.2.4; P-65.1.7.3.3
trithiophosphono*	$(HS)_2P(S)$–	P-67.1.4.1.1.1
trithiosulfo* = sulfanylsulfonodithioyl	$HS\text{-}S(S)_2$–	P-65.3.2.1
trityl (unsubstituted) = triphenylmethyl*	$(C_6H_5)_3C$–	P-29.6.2.2
undecan-1-yl = undecyl*	$CH_3\text{-}[CH_2]_9\text{-}CH_2$–	P-29.3.2.1; P-29.3.2.2
undecyl* = undecan-1-yl	$CH_3\text{-}[CH_2]_9\text{-}CH_2$–	P-29.3.2.1; P-29.3.2.2
ureido: see carbamoylamino*		
ureylene: see carbonylbis(azanediyl)*		
vinyl = ethenyl*	CH_2=CH–	P-32.3
vinylidene: see ethenylidene*		
vinylidene = ethenylidene*	CH_2=C=	P-32.3
2,3-xylidino: see 2,3-dimethylanilino*		

yloamino* = yloazanyl	$HN^{\bullet}–$	P-71.5
yloazanyl = yloamino*	$HN^{\bullet}–$	P-71.5
yloformyl*	$O=C^{\bullet}–$	P-71.5
ylohydroxy: see ylooxidanyl*		
ylomethyl*	$H_2C^{\bullet}–$	P-71.5
ylooxidanyl* = ylooxy (not ylohydroxy)	$^{\bullet}O–$	P-71.5
(ylooxidanyl)formyl = oxylcarbonyl*	$^{\bullet}O\text{-}CO–$	P-71.5
ylooxy = ylooxidanyl* (not ylohydroxy)	$^{\bullet}O–$	P-71.5

International Union of Pure and Applied Chemistry

Division VIII Chemical Nomenclature and Structure Representation Division

Nomenclature of Organic Chemistry. IUPAC Recommendations and Preferred Names 2013.

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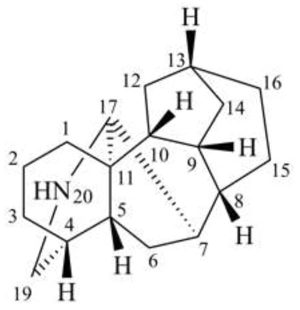
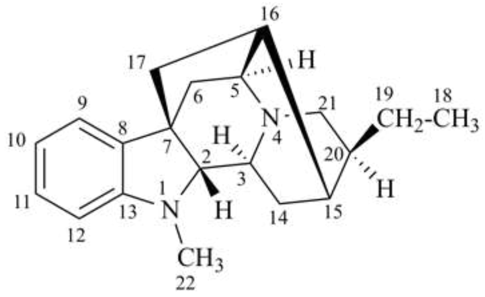
Royal Society of Chemistry, ISBN 978-0-85404-182-4

Appendix 3. STRUCTURES FOR ALKALOIDS, STEROIDS, TERPENOIDS, AND SIMILAR COMPOUNDS

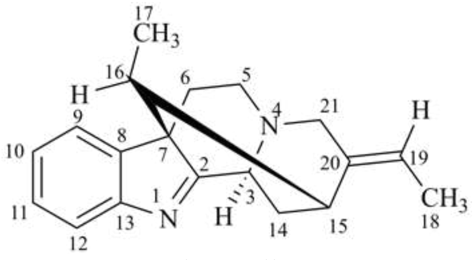
1. Alkaloids


H
13
12
16
17
H
14
1
H
2
10
9
15
11
HN20
5
8
3
4
7
H
H
6
19
H

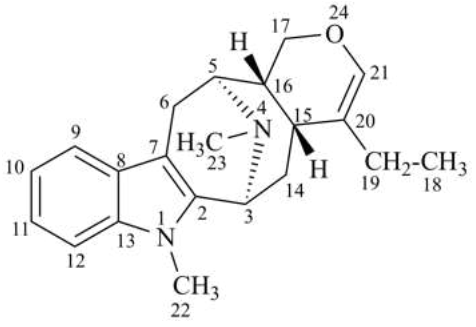
aconitane


16
H
17
19
18
9
6
5
21
CH_2-CH_3
N
10
8
H
4
20
7
2
3
1
11
13
N
H
14
15
H
12
CH_3
22

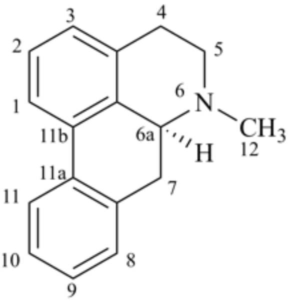
ajmalan


17
CH_3
16
6
5
H
H
4
21
9
N
10
8
7
2
20
19
1
3
11
13
N
H
14
15
CH_3
12
18

akuammilan
(named systematically by CAS)

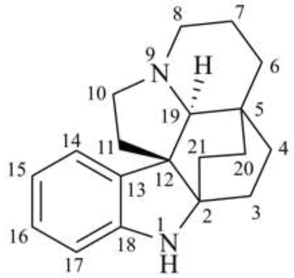

24
H
17
O
5
21
16
6
4
15
20
9
7
H_3C
N
23
10
8
H
CH_2-CH_3
14
19
18
2
3
1
11
13
N
12
CH_3
22

alstophyllan
(named systematically by CAS)



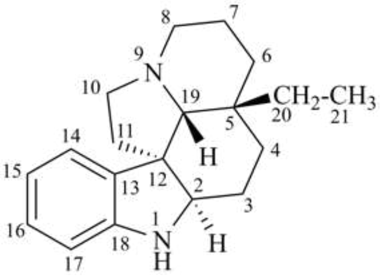
3
4
2
5
6
N
1
CH3
11b
6a
H
12
11a
7
11
10
8
9

aporphine
(named systematically by CAS)



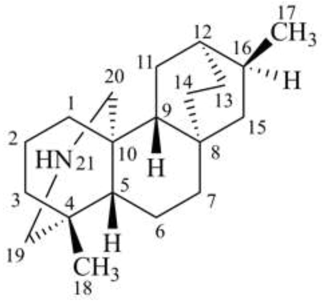
8
7
9
N
H
6
10
19
5
14
11
21
4
15
12
20
13
16
1
2
3
18
N
H
17

aspidofractinine
(named systematically by CAS)



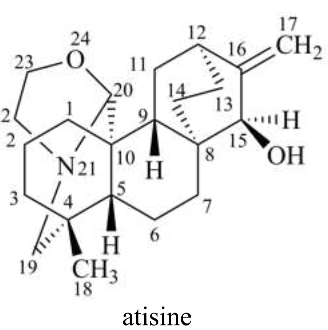
8
7
9
N
6
10
19
CH2-CH3
20
21
11
5
14
H
4
15
12
13
2
3
16
1
18
N
H
H
17

aspidospermidine



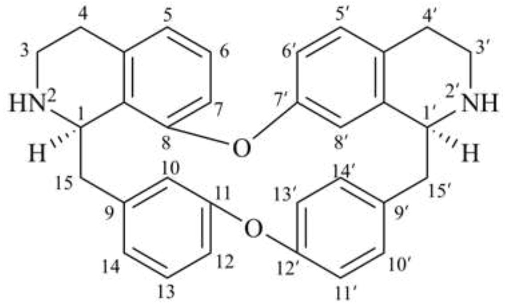
17
12
CH3
11
16
H
20
14
13
1
9
15
2
HN21
10
8
H
3
4
5
7
6
19
H
CH3
18

atidane
(named systematically by CAS)

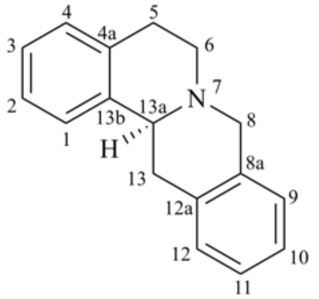


24
12
17
23
O
11
16
CH2
20
14
22
13
1
9
H
2
15
N21
10
8
H
OH
3
5
7
4
H
6
19
CH3
18

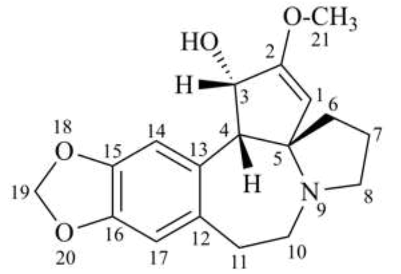
atisine
(named systematically by CAS)


4
5
5′
4′
3
6
6′
3′
2′
HN
2
NH
1
7
7′
1′
H
8
O
8′
H
10
14′
15
11
13′
15′
9
O
9′
14
12
12′
10′
13
11′

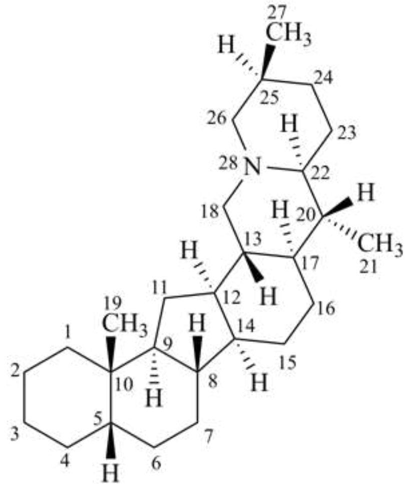
berbaman
(named systematically by CAS)


4
5
4a
3
6
N
7
2
13b
13a
8
1
H
8a
13
9
12a
12
10
11

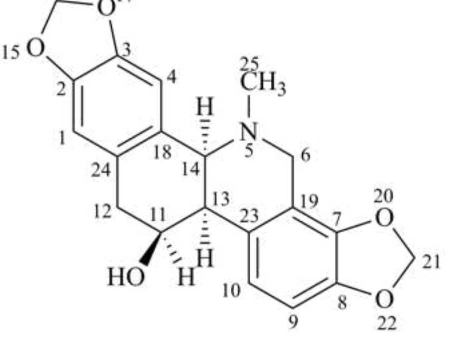
berbine
(named systematically by CAS)


O-CH3
HO
2
21
H
3
1
6
18
14
13
4
7
O
15
5
19
H
N
9
8
O
16
12
20
17
11
10

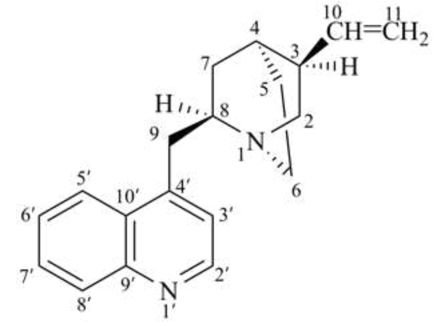
cephalotaxine


27
CH3
H
25
24
26
H
23
28
N
22
H
18
H
20
CH3
H
13
17
21
11
H
19
12
16
1
CH3
9
H
14
2
10
H
8
H
15
3
5
7
4
H
6

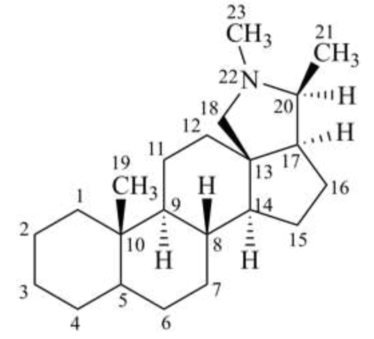
cevane


16
O
17
15
O
3
4
25
CH3
2
H
N
1
5
6
18
14
24
20
13
19
7
O
12
11
23
21
HO
H
H
O
10
8
9
22

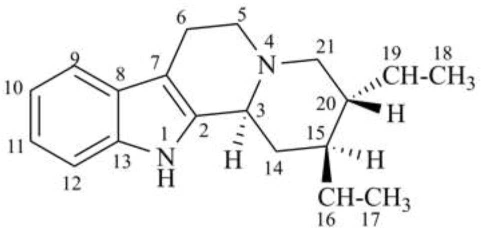
chelidonine
(named systematically by CAS)


CH=CH$_2$
H
N
N
1′
2′
3′
4′
5′
6′
7′
8′
9′
10′
1
2
3
4
5
6
7
8
9
10
11

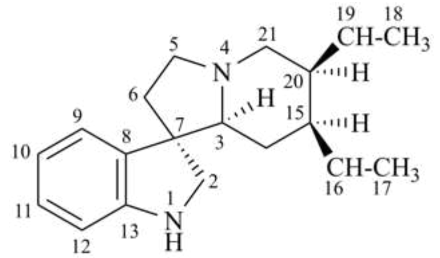
cinchonan


CH$_3$
CH$_3$
CH$_3$
N
H
1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17
18
19
20
21
22
23

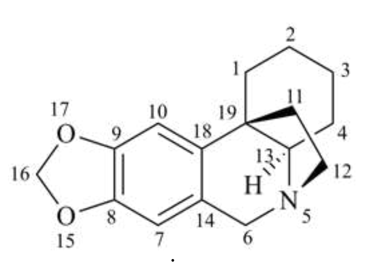
conanine


N
NH
H
CH-CH$_3$
CH-CH$_3$
1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17
18
19
20
21

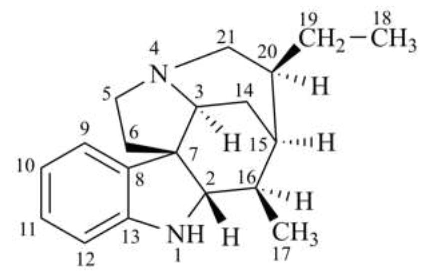
corynan
(named systematically by CAS)


N
NH
H
CH-CH$_3$
CH-CH$_3$
1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17
18
19
20
21

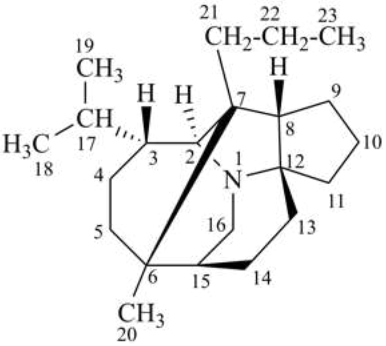
corynoxan
(named systematically by CAS)


O
O
N
H
1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17
18
19

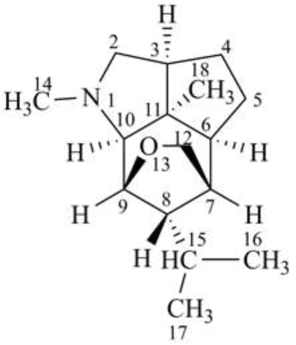
crinan
(named systematically by CAS)


CH$_2$−CH$_3$
CH$_3$
N
NH
H
1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17
18
19
20
21

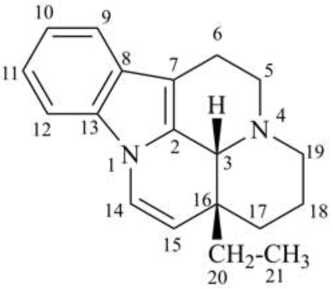
curan



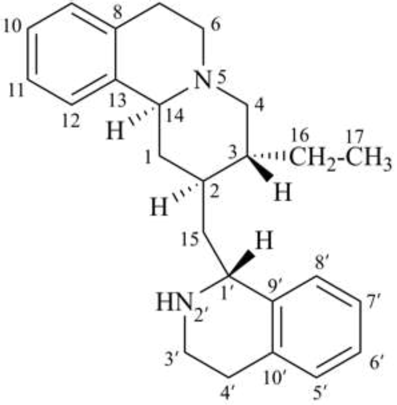
daphnane
(named systematically by CAS)



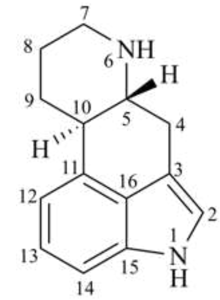
dendrobane
(named systematically by CAS)



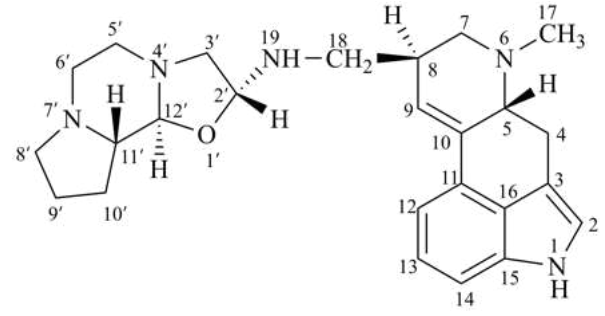
eburnamenine



emetan
(named systematically by CAS)

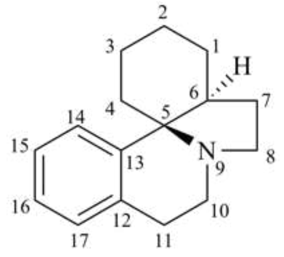


ergoline



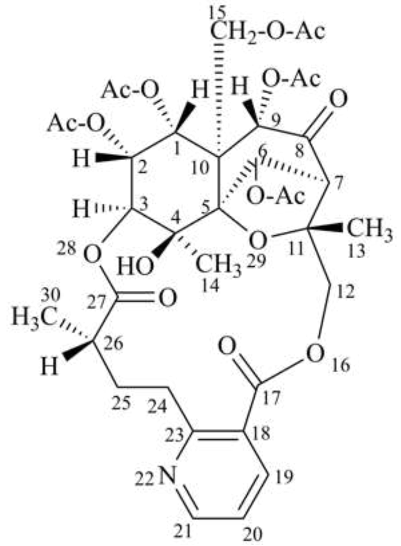
19
NH
18
CH2
H
7
17
6
N
CH3
H
5
4
8
9
10
11
16
3
2
1
NH
15
14
13
12
5′
6′
4′
N
3′
2′
H
7′
N
H
12′
O
1′
11′
H
8′
9′
10′

ergotaman



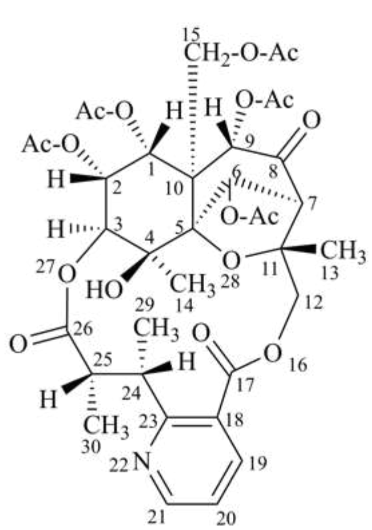
2
3
1
H
4
6
7
5
14
15
13
N
9
8
16
12
10
17
11

erythrinan



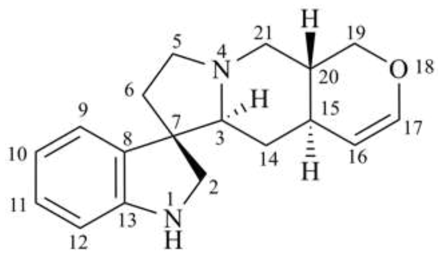
15
CH2-O-Ac
Ac-O
H
H
O-Ac
O
Ac-O
1
9
8
H
2
10
6
O-Ac
7
H
3
5
4
O
11
CH3
13
28
O
HO
CH3
14
29
30
27
O
12
H3C
26
H
O
O
16
17
25
24
23
18
22
N
19
21
20

evonimine
(named systematically by CAS)

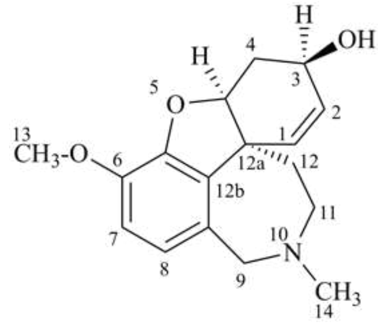


15
CH2-O-Ac
Ac-O
H
H
O-Ac
O
Ac-O
1
9
8
H
2
10
6
O-Ac
7
H
3
5
4
O
11
CH3
13
27
O
HO
CH3
14
28
29
12
CH3
26
O
H
O
16
25
24
17
H
CH3
23
18
30
22
N
19
21
20

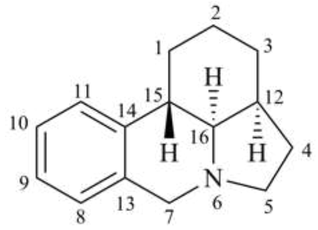
evonine
(named systematically by CAS)


H
21
19
5
4
N
20
O
18
6
H
15
9
7
17
3
10
8
14
16
H
2
1
11
N
13
H
12

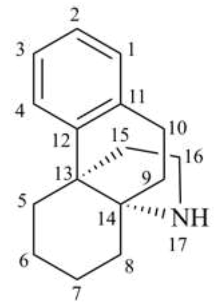
formosanan
(named systematically by CAS)


H
OH
H
4
3
5
O
2
1
13
CH3-O
6
12a
12
12b
11
10
7
N
8
9
CH3
14

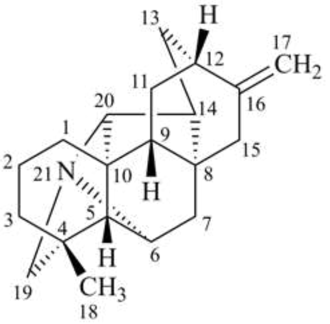
galanthamine
(named systematically by CAS)


2
1
3
H
11
15
12
14
10
16
H
H
4
N
9
13
6
7
5
8

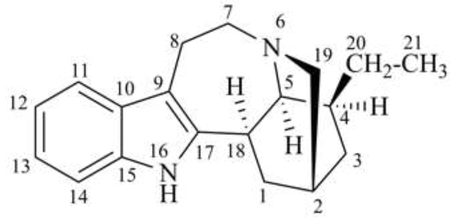
galanthan
(named systematically by CAS)


2
3
1
11
4
10
12
15
16
9
13
5
14
NH
17
6
8
7

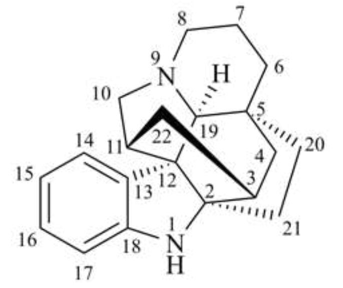
hasubanan


13
H
17
12
CH2
11
20
14
16
1
9
2
21
N
10
15
8
H
5
3
4
7
H
6
19
CH3
18

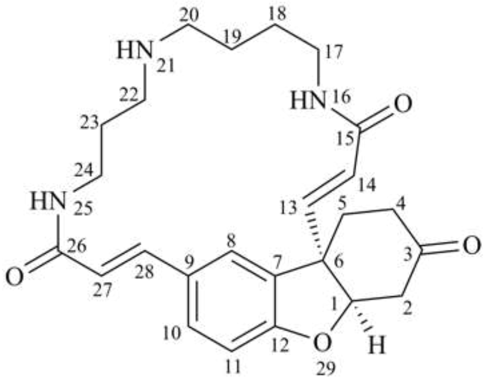
hetisan


7
6
8
N
19
20
21
CH2-CH3
11
10
9
H
5
12
4
H
H
13
16
17
18
3
15
N
H
1
14
2

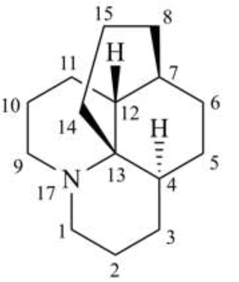
ibogamine


8
7
9
N
H
6
10
5
22
19
11
14
20
4
15
13
12
3
2
1
21
16
18
NH
H
17

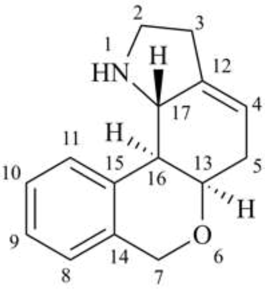
kopsan
(named systematically by CAS)


20
18
19
HN
21
17
22
HN
16
O
23
15
14
24
HN
25
13
5
4
26
9
8
3
O
7
6
O
27
28
1
2
10
12
O
H
11
29

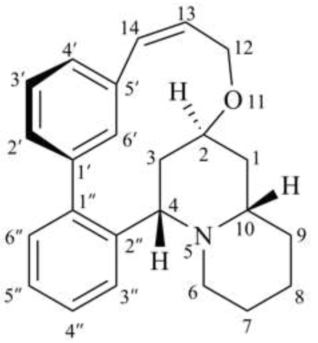
lunarine
(named systematically by CAS)


15
8
11
H
7
10
12
6
14
H
9
5
13
17
N
4
1
3
2

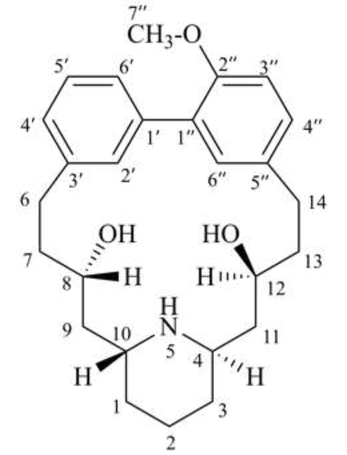
lycopodane
(named systematically by CAS)


2
3
1
HN
H
12
4
17
H
11
5
13
10
15
16
H
9
O
6
8
14
7

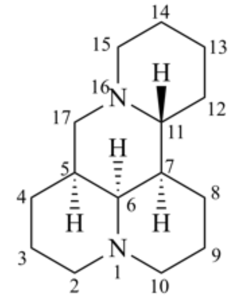
lycorenan
(named systematically by CAS)


14
13
4′
12
3′
5′
H
O
11
2′
6′
3
2
1
1′
H
1″
4
10
6″
2″
N
5
9
H
5″
3″
6
8
4″
7

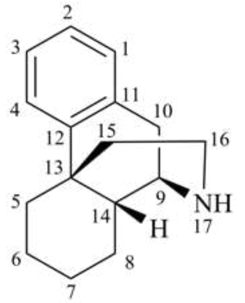
lythran
(named systematically by CAS)


7″
CH3-O
2″
3″
4″
5″
6″
1″
1′
2′
3′
4′
5′
6′
6
7
8
9
10
OH
H
HO
H
12
13
14
11
H
N
5
4
H
H
1
2
3

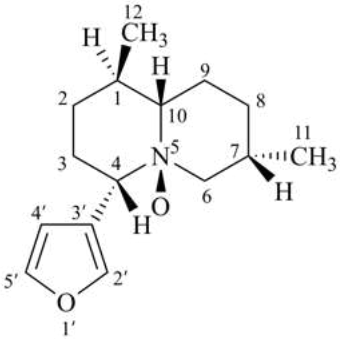
lythranidine
(named systematically by CAS)


14
15
13
16
N
H
12
17
11
H
5
7
8
4
6
H
H
3
N
9
2
1
10

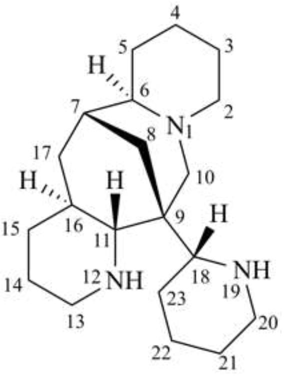
matridine
(named systematically by CAS)


2
3
1
11
4
10
12
15
16
13
9
5
NH
14
H
17
6
8
7

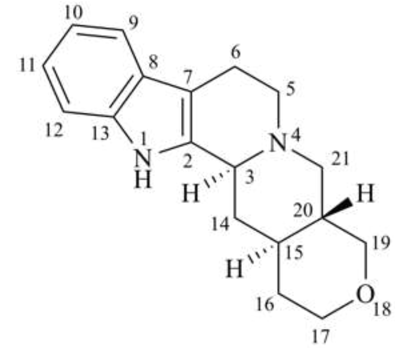
morphinan


12
H
CH3
H
9
2
1
8
10
11
3
4
N
5
7
CH3
O
6
H
4′
3′
H
5′
O
2′
1′

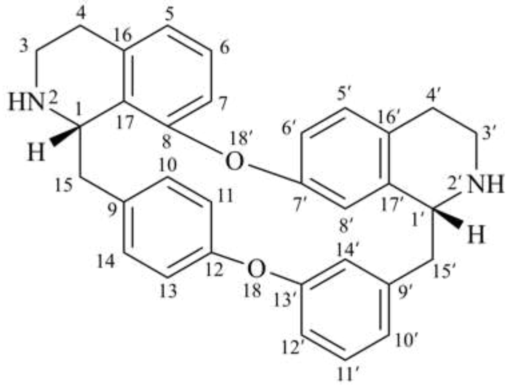
nupharidine
(named systematically by CAS)


H
N1
H
H
12NH
H
NH
19

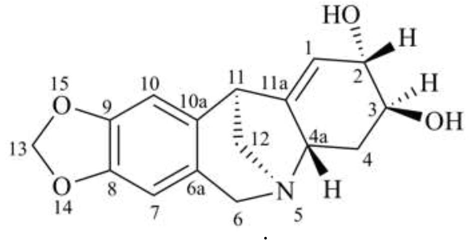
ormosanine
(named systematically by CAS)


N
H
N4
H
H
H
O18

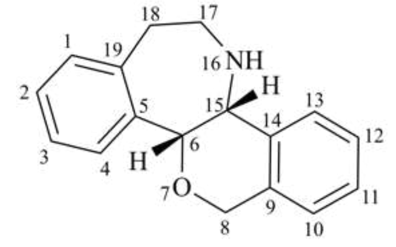
18-oxayohimban


HN2
H
O
18′
O
18
2′NH
H

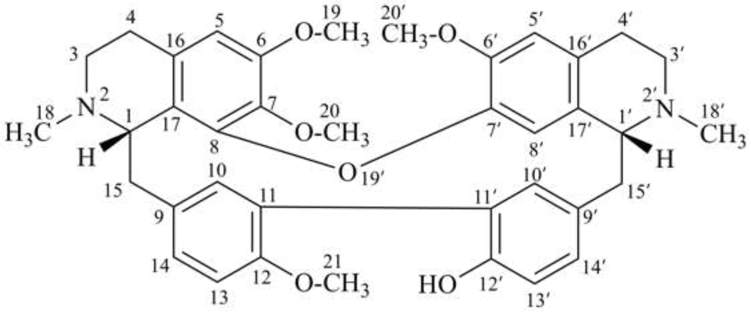
oxyacanthan
(named systematically by CAS)


HO
H
H
OH
O
15
O
14
N
5
H

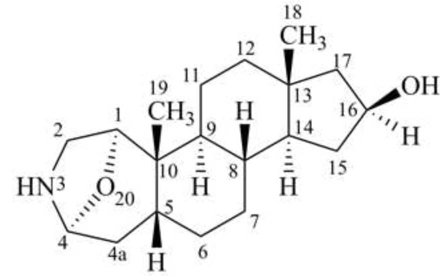
pancracine
(named systematically by CAS)



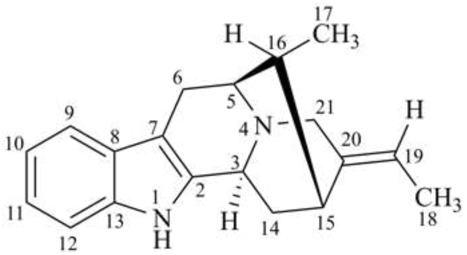
rheadan
(named systematically by CAS)


O-CH3
CH3-O
O-CH3
H3C
N
H
O
N
CH3
H
O-CH3
HO

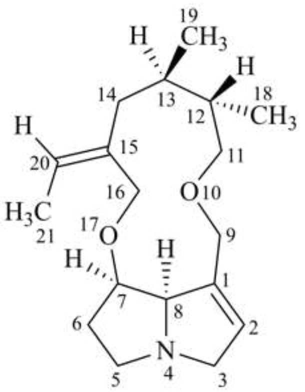
rodiasine
(named systematically by CAS)


CH3
OH
CH3
H
HN
O
H
H
H
H

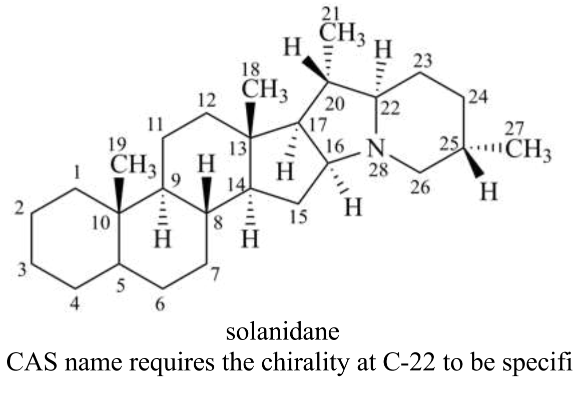
samandarine
(named systematically by CAS)


H
CH3
H
N
N
H
H
CH3

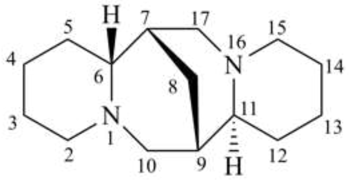
sarpagan


H
CH3
H
CH3
H
O
H3C
O
H
H
N

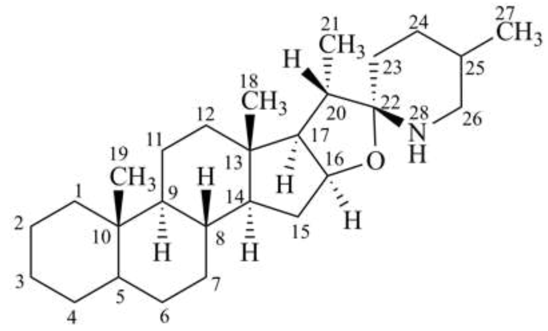
senecionan
(named systematically by CAS)


CH3
H
H
CH3
CH3
N
CH3
H
H
H
H
H
H

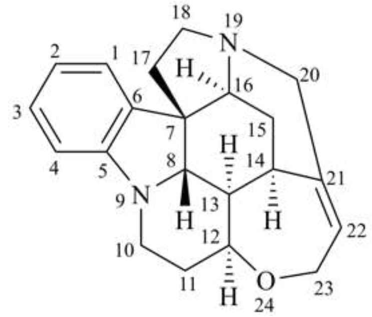
solanidane
(the CAS name requires the chirality at C-22 to be specified)


H
7
17
15
5
16
4
N
14
6
8
N
11
3
1
13
2
10
9
12
H

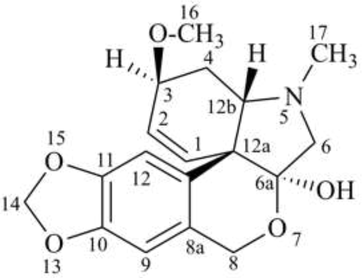
sparteine
(named systematically by CAS)


21
CH3
24
27
CH3
H
23
25
18
CH3
22
28
20
26
12
NH
H
17
19
11
13
16
O
CH3
9
H
H
14
1
H
2
10
8
15
H
H
H
3
7
5
4
6

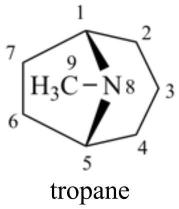
spirosolane
(the CAS name requires the chirality at C-22 to be specified)


18
19
N
2
1
17
H
20
16
6
3
15
7
H
14
8
4
21
5
13
N
9
H
H
22
12
10
11
O
23
H
24

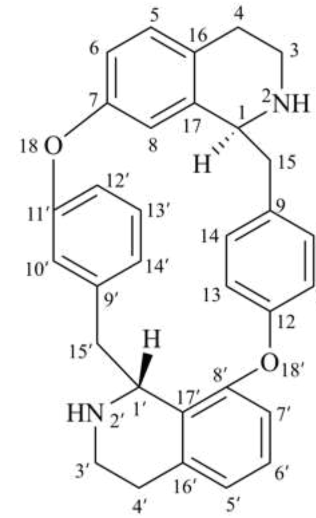
strychnidine


16
O-CH3
17
H
CH3
H
4
N
3
12b
5
2
15
12a
6
1
11
O
12
6a
OH
14
O
O
7
10
9
8a
8
13

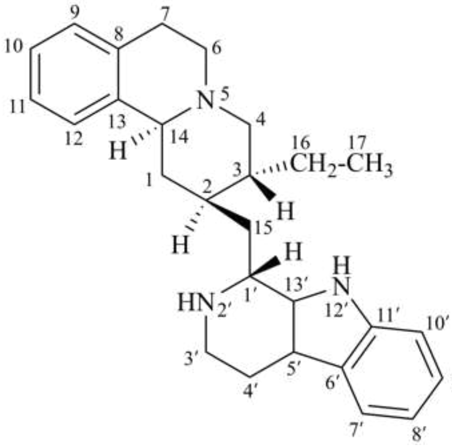
tazettine
(named systematically by CAS)


1
2
7
9
H3C
N
8
3
6
4
5

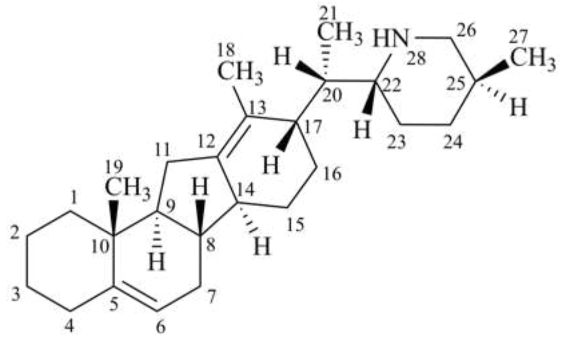
tropane
(named systematically by CAS)


NH
O
H
HN
O
1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17
18
1′
2′
3′
4′
5′
6′
7′
8′
9′
10′
11′
12′
13′
14′
15′
16′
17′
18′

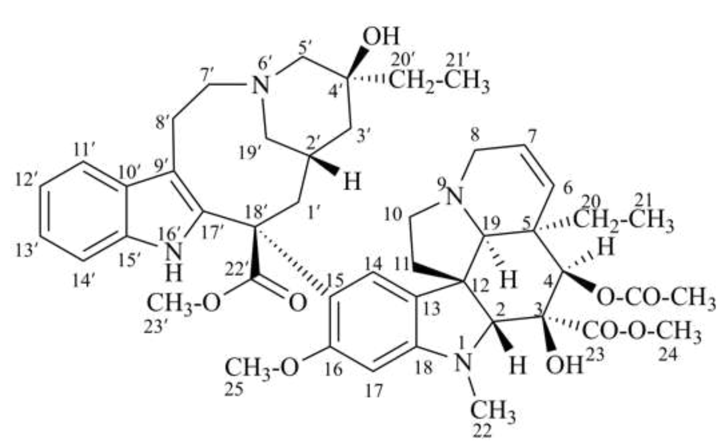
tubocuraran
(named systematically by CAS)


N
H
H
H
CH$_2$-CH$_3$
H
HN
H
N
1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17
1′
2′
3′
4′
5′
6′
7′
8′
9′
10′
11′
12′
13′

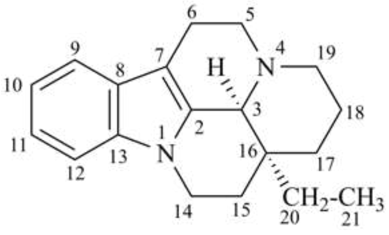
tubulosan
(named systematically by CAS)


CH$_3$
HN
CH$_3$
H
H
H
H
CH$_3$
H
H
H
H
CH$_3$
1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17
18
19
20
21
22
23
24
25
26
27
28

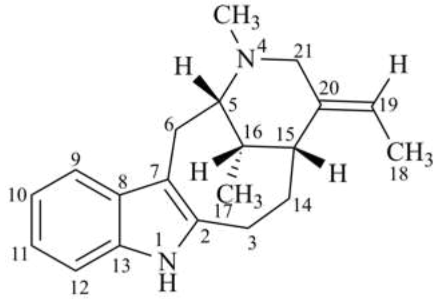
veratraman
(named systematically by CAS)


OH
N
CH$_2$-CH$_3$
H
NH
CH$_3$-O
O
N
CH$_2$-CH$_3$
H
H
O-CO-CH$_3$
CO-O-CH$_3$
OH
H
N
CH$_3$-O
CH$_3$
1′
2′
3′
4′
5′
6′
7′
8′
9′
10′
11′
12′
13′
14′
15′
16′
17′
18′
19′
20′
21′
22′
23′
1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17
18
19
20
21
22
23
24
25

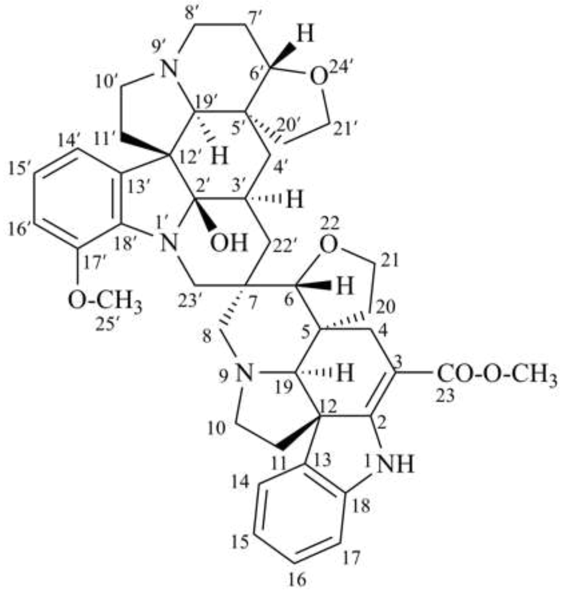
vincaleukoblastine


6
5
9
7
4
19
8
H
N
10
3
18
2
1
11
13
N
16
17
12
CH2-CH3
14
15
20
21

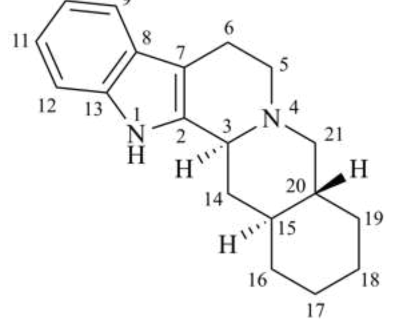
vincane
(CAS name based on eburnamenine)


CH3
N
4
21
H
H
20
19
5
6
16
15
9
7
H
CH3
H
18
8
CH3
10
17
14
2
3
11
1
13
N
H
12

vobasan

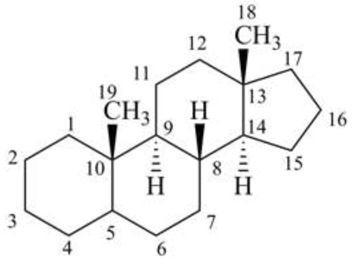

8′
7′
H
9′
N
6′
O
24′
10′
19′
5′
20′
21′
14′
11′
12′
H
4′
15′
13′
2′
3′
H
22
16′
1′
N
OH
22′
O
21
18′
17′
H
23′
7
6
20
O-CH3
25′
8
5
4
9
N
H
3
CO-O-CH3
19
23
2
10
12
11
13
1
NH
14
18
15
17
16

vobtusine
(named systematically by CAS)

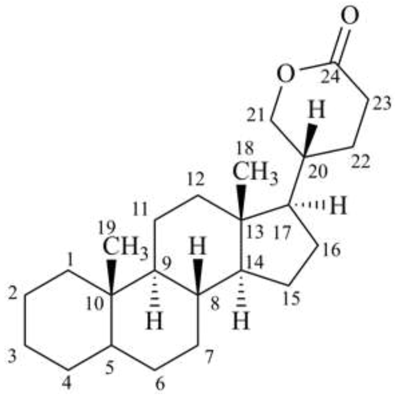

10
9
6
11
8
7
5
12
13
N
4
1
2
3
21
N
H
H
20
H
19
14
H
15
16
18
17

yohimban

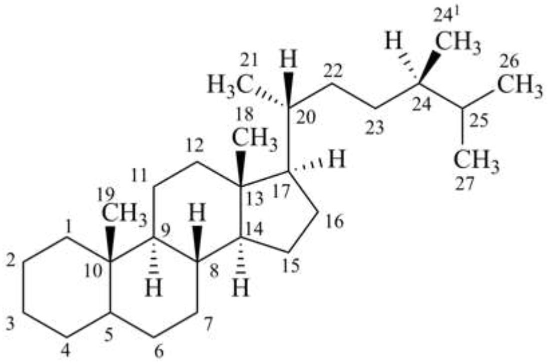
2. Steroids


18
CH3
12
17
11
13
19
CH3
H
16
1
9
14
2
10
8
15
H
H
3
5
7
4
6

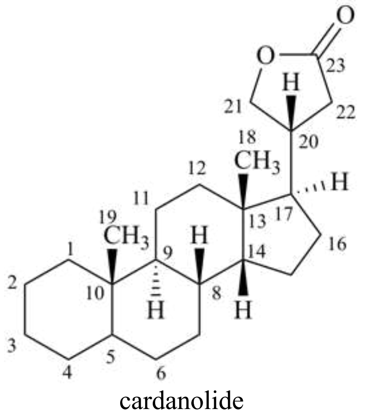
androstane


O
O
24
23
21
H
22
20
18
CH3
12
H
11
17
13
19
CH3
16
1
H
9
14
2
10
8
15
H
H
3
7
5
4
6

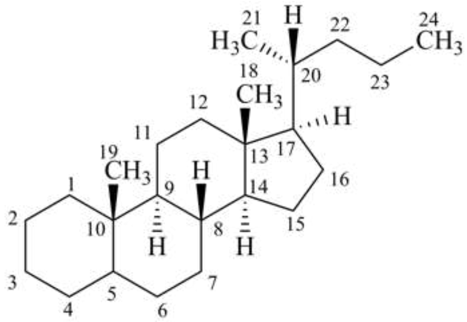
bufanolide


24¹
H
CH3
21
H
22
26
H3C
CH3
24
20
18
25
23
CH3
12
H
CH3
27
11
17
13
19
CH3
H
16
1
9
14
2
10
8
15
H
H
3
7
5
4
6

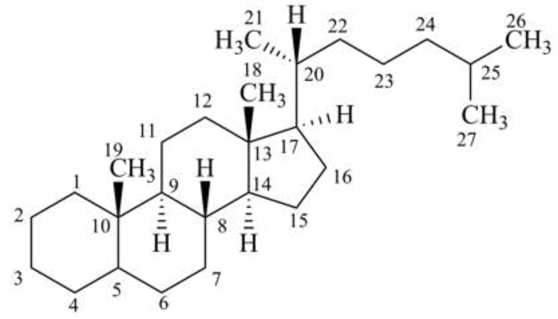
campestane
(named by CAS as a stereoisomer of ergostane in which the locant 24^1 is 28)


O
O
23
H
21
22
20
18
12
CH3
H
11
17
13
19
CH3
16
1
H
9
14
2
10
8
H
H
3
5
4
6

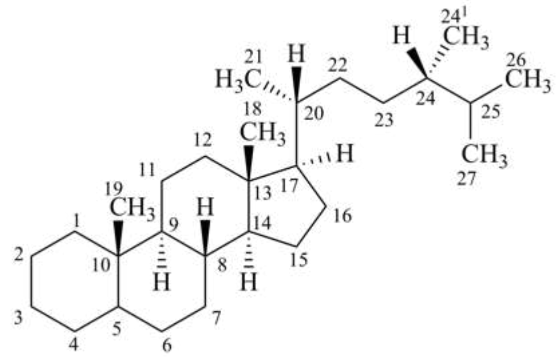
cardanolide


21
H
22
24
H3C
CH3
20
18
23
12
CH3
H
11
17
13
19
CH3
H
16
1
9
14
2
10
8
15
H
H
3
7
5
4
6

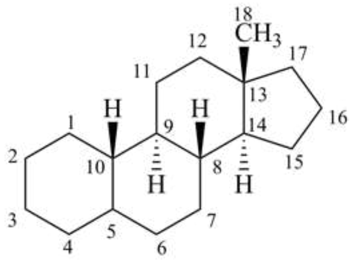
cholane



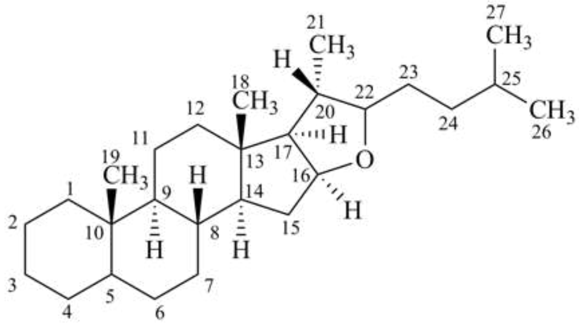
cholestane



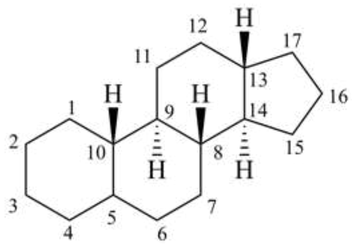
ergostane



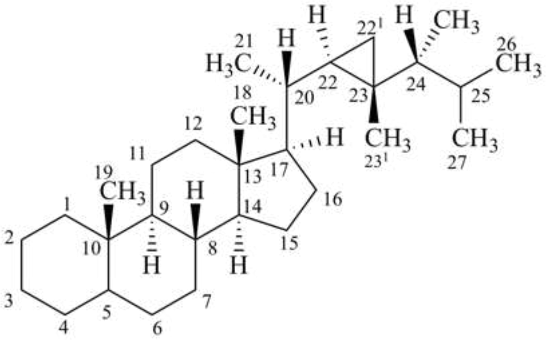
estrane



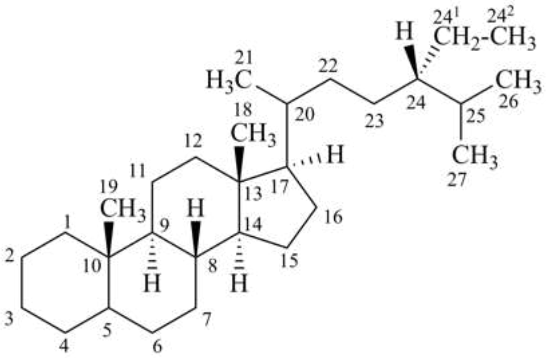
furostan



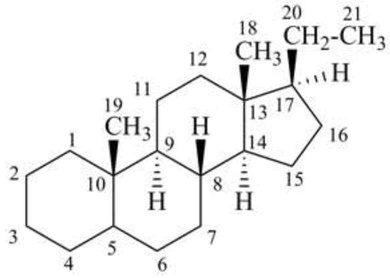
gonane



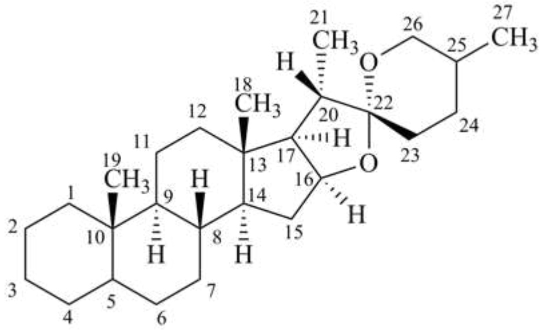
gorgostane
(for CAS the locants 22^1, 23^1, and 24^1 are 34, 33, and 28, respectively)



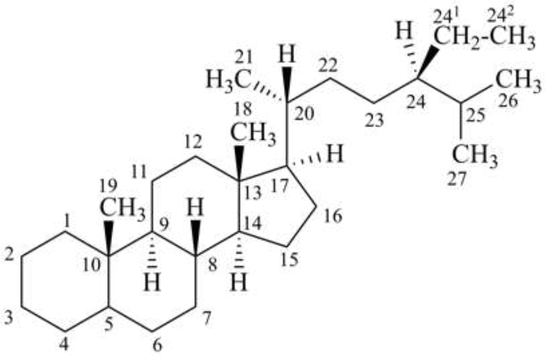
poriferastane
(named by CAS as a stereoisomer of stigmastane in which the locants 24^1 and 24^2 are 28 and 29, respectively.)



pregnane

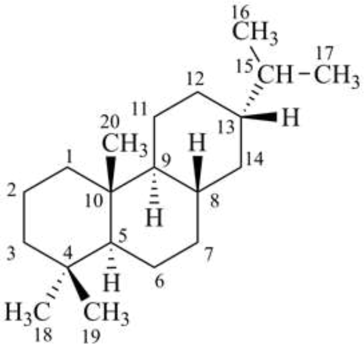


spirostan
(the CAS name requires the chirality at C-22 to be specified)



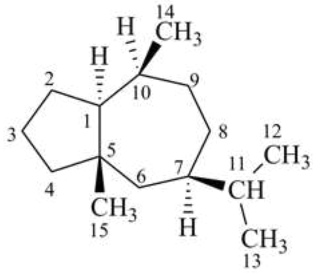
stigmastane

3. Terpenoids



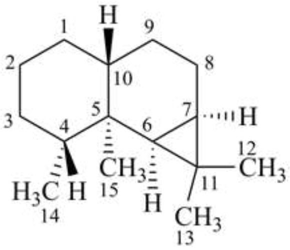
16
CH3
17
15 CH−CH3
12
11
13
H
20
CH3
H
9
14
1
2
10
8
H
3
4
5
7
H
6
H3C
CH3
18
19

abietane
(named systematically by CAS)



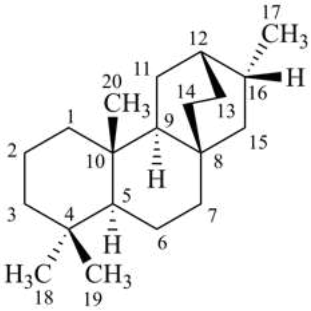
H
14
CH3
H
2
10
9
3
1
8
12
5
11
CH3
4
6
7
CH
CH3
15
H
CH3
13

ambrosane
(named systematically by CAS)



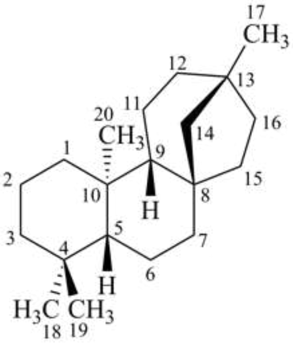
1
H
9
2
8
10
5
7
H
3
4
6
12
CH3
CH3
11
H3C
H
15
H
14
CH3
13

aristolane
(named systematically by CAS)



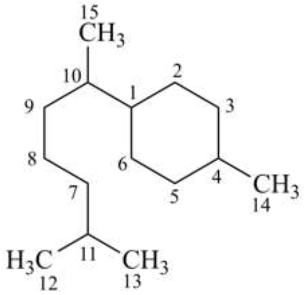
17
CH3
12
11
H
20
14
16
CH3
13
1
9
15
2
10
8
H
3
4
5
7
H
6
H3C
CH3
18
19

atisane



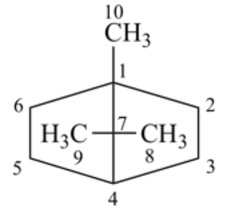
17
CH3
12
13
20
11
16
CH3
14
1
9
2
10
15
H
8
5
3
7
4
6
H
H3C
CH3
18
19

beyerane
(CAS name based on kaurane)



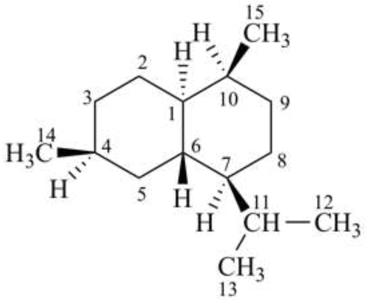
15
CH3
10
1
2
3
4
CH3
14
5
6
9
8
7
11
H3C
12
CH3
13

bisabolane
(named systematically by CAS)



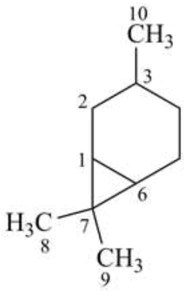
10
CH3
1
2
3
4
5
6
7
H3C
9
CH3
8

bornane
(named systematically by CAS)



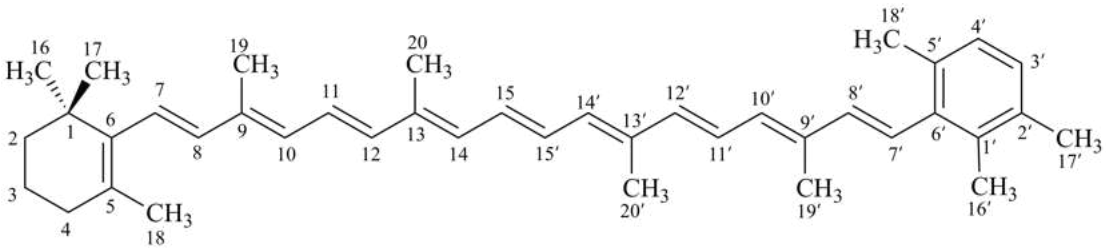
15
H
CH3
2
3
1
10
9
14
H3C
4
6
7
8
H
5
H
H
11
CH
12
CH3
CH3
13

cadinane
(named systematically by CAS)



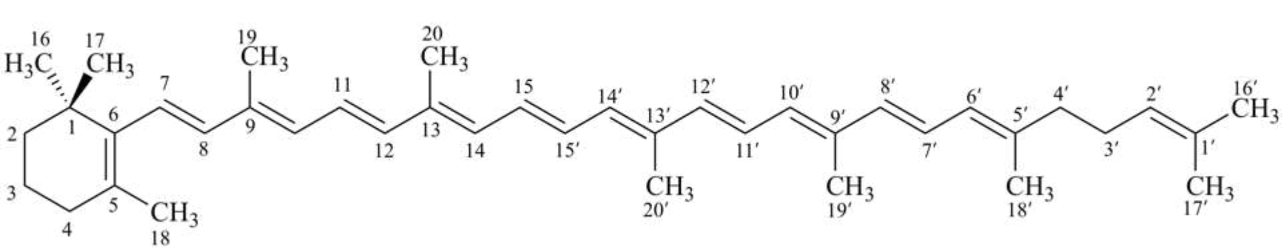
10
CH3
3
2
4
1
5
6
H3C
7
8
CH3
9

carane
(named systematically by CAS)



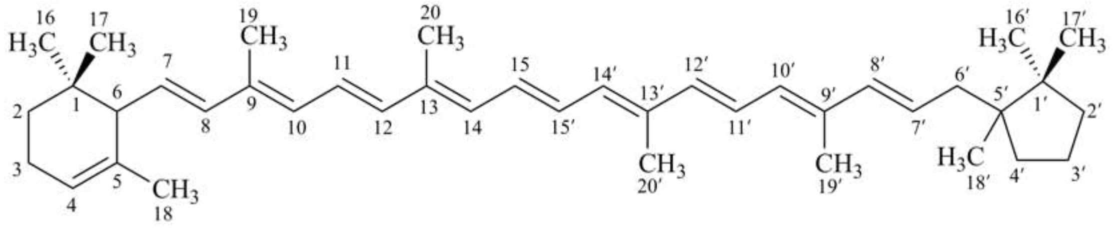
16
17
H3C
CH3
1
2
3
4
5
6
CH3
18
7
8
19
CH3
9
10
11
12
20
CH3
13
14
15
15′
14′
13′
CH3
20′
12′
11′
10′
9′
CH3
19′
8′
7′
6′
18′
H3C
5′
4′
3′
2′
CH3
17′
1′
CH3
16′

β,φ-carotene

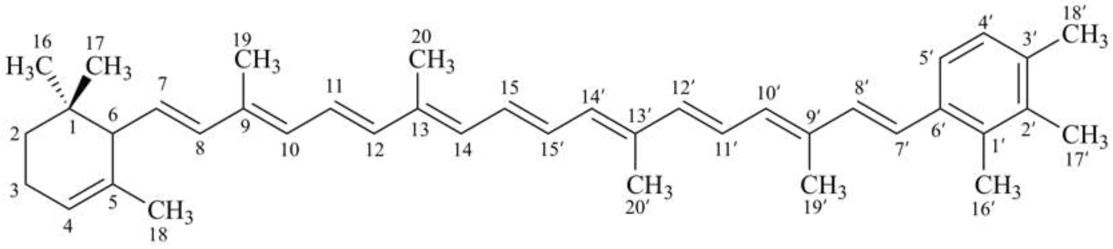


16
17
H3C
CH3
1
2
3
4
5
6
CH3
18
7
8
19
CH3
9
10
11
12
20
CH3
13
14
15
15′
14′
13′
CH3
20′
12′
11′
10′
9′
CH3
19′
8′
7′
6′
5′
CH3
18′
4′
3′
2′
1′
16′
CH3
CH3
17′

β,ψ-carotene

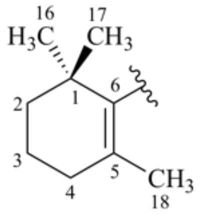

H_3C 16
17 CH_3
19 CH_3
20 CH_3
CH_3 18
CH_3 20′
CH_3 19′
H_3C 16′
17′ CH_3
H_3C 18′

ε,κ-carotene

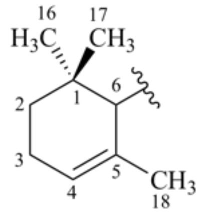

H_3C 16
17 CH_3
19 CH_3
20 CH_3
CH_3 18
CH_3 20′
CH_3 19′
18′ CH_3
CH_3 17′
CH_3 16′

ε,χ-carotene

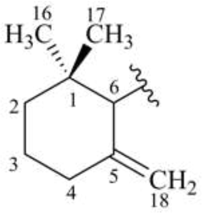
Note: There are 28 possible carotene parent structures of which four are illustrated above.
The 28 are derived from all permutations of the following seven end groups:


H_3C 16
17 CH_3
CH_3 18

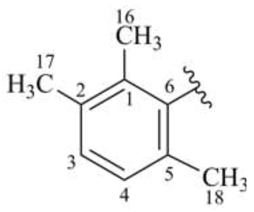
β (beta)


H_3C 16
17 CH_3
CH_3 18

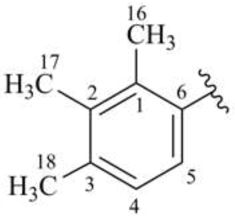
ε (epsilon)


H_3C 16
17 CH_3
CH_2 18

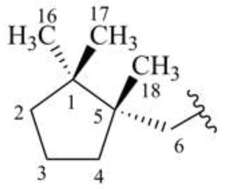
γ (gamma)


16 CH_3
17 H_3C
CH_3 18

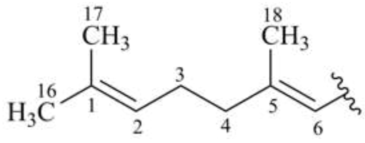
φ (phi)


16 CH_3
17 H_3C
18 H_3C

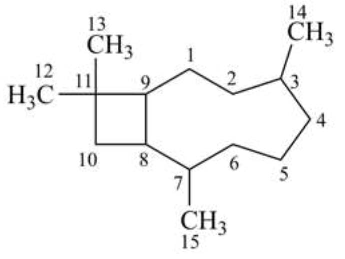
χ (chi)


H_3C 16
17 CH_3
CH_3 18

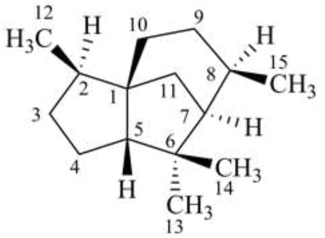
κ (kappa)


17 CH_3
18 CH_3
H_3C 16

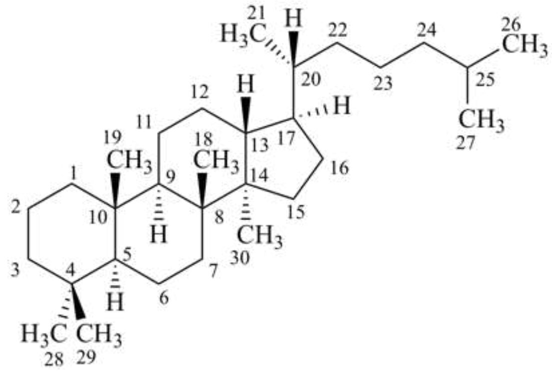
ψ (psi)


13 CH_3
12 H_3C
14 CH_3
CH_3 15

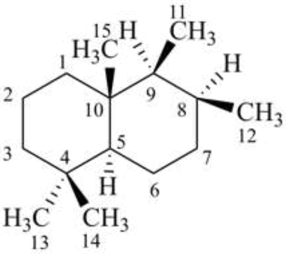
caryophyllane
(named systematically by CAS)


12 H_3C
H
H
15 CH_3
H
CH_3 14
H
CH_3 13

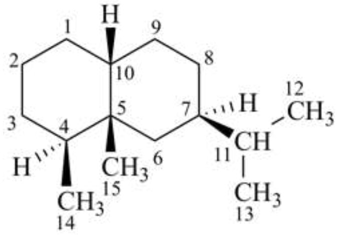
cedrane
(named systematically by CAS)


21
H
H_3C
22
24
26
CH_3
20
23
25
12
H
H
17
CH_3
27
11
19
18
13
CH_3
CH_3
16
1
9
14
2
10
8
15
H
CH_3
3
4
5
7
30
H
6
H_3C
CH_3
28
29

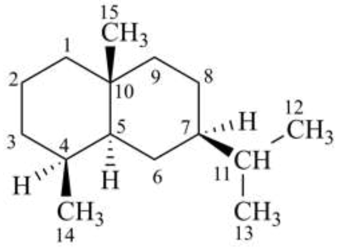
dammarane


11
15
H
CH_3
H_3C
H
1
9
2
8
10
CH_3
12
5
3
7
4
H
6
H_3C
CH_3
13
14

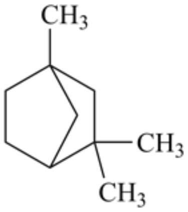
drimane
(named systematically by CAS)


H
1
9
2
8
10
12
CH_3
5
7
H
3
4
CH
11
H
6
CH_3
15
CH_3
CH_3
14
13

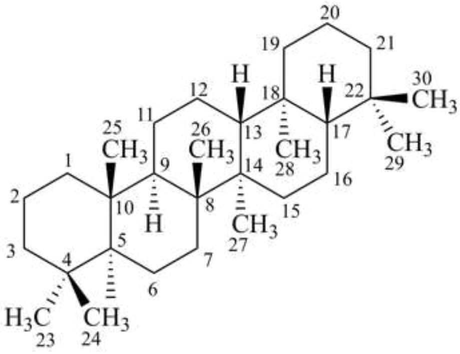
eremophilane
(named systematically by CAS)


15
CH_3
1
9
8
2
10
12
5
7
H
CH_3
3
4
CH
11
H
H
6
CH_3
CH_3
14
13

eudesmane
(named systematically by CAS)

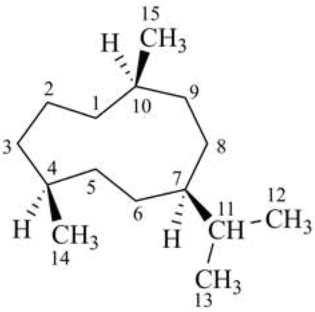


fenchane
(named systematically by CAS)



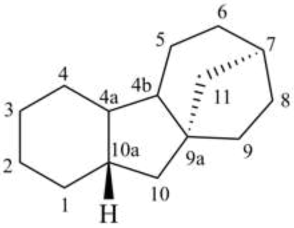
20
19
21
H
H
30
12
18
22
CH3
11
13
17
25
26
CH3
CH3
CH3
28
29
1
9
14
16
2
10
8
15
H
CH3
5
27
3
7
4
6
H3C
CH3
23
24

gammacerane



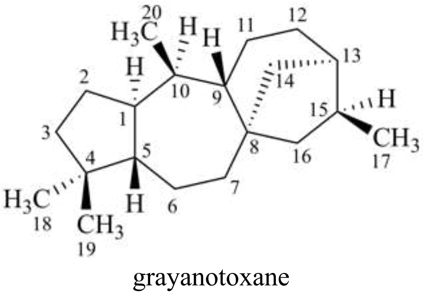
15
H
CH3
2
1
10
9
3
8
4
5
7
12
6
11
H
CH3
H
CH
CH3
14
CH3
13

germacrane
(named systematically by CAS)



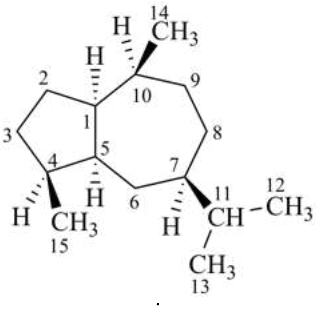
6
5
7
4
4b
4a
11
8
3
10a
9a
9
2
1
10
H

gibbane



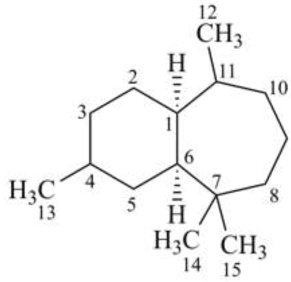
20
H3C
H
H
11
12
H
13
2
10
9
14
15
H
1
3
8
5
16
CH3
17
4
7
H3C
H
6
18
CH3
19

grayanotoxane



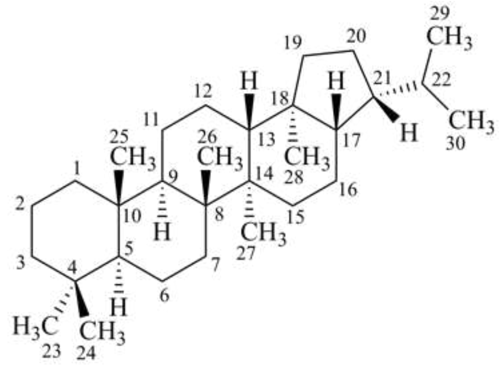
14
H
CH3
H
2
10
9
1
3
8
5
4
7
12
H
6
11
H
CH3
H
CH
CH3
15
CH3
13

guaiane
(named systematically by CAS)



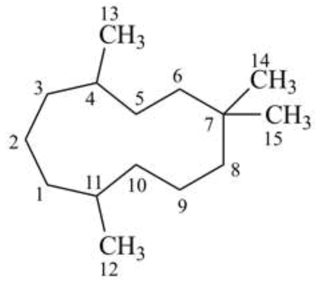
12
CH3
H
2
11
10
3
1
9
6
H3C
4
7
8
13
5
H
H3C
CH3
14
15

himachalane
(named systematically by CAS)



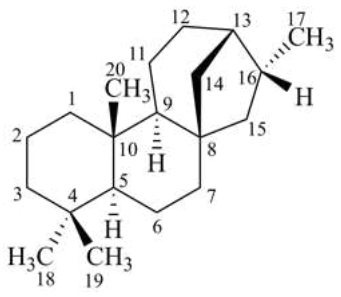
29
19
20
CH3
H
21
22
12
H
18
11
13
H
CH3
25
26
17
30
CH3
CH3
CH3
1
9
14
28
16
2
10
8
15
H
CH3
3
4
5
7
27
H
6
H3C
CH3
23
24

hopane
(CAS name based on gammacerane)



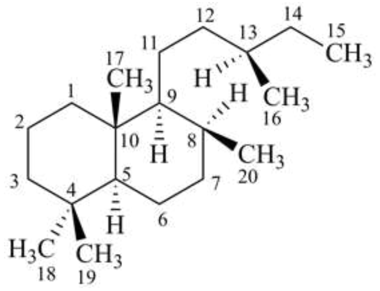
13
CH3
14
6
CH3
3
4
5
7
CH3
15
2
8
11
10
1
9
CH3
12

humulane
(named systematically by CAS)



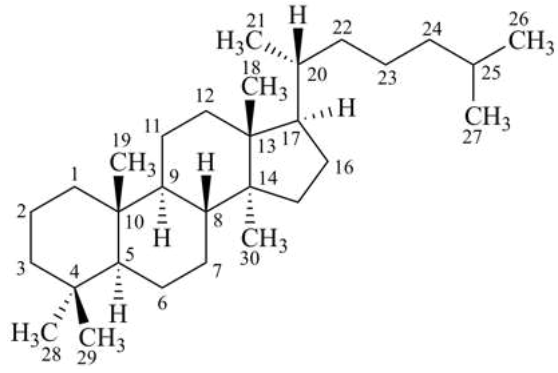
12
13
17
CH3
11
20
16
CH3
14
H
1
9
2
15
10
H
8
5
3
4
7
H
6
H3C
CH3
18
19

kaurane
(named by CAS *ent*-stereoisomer)

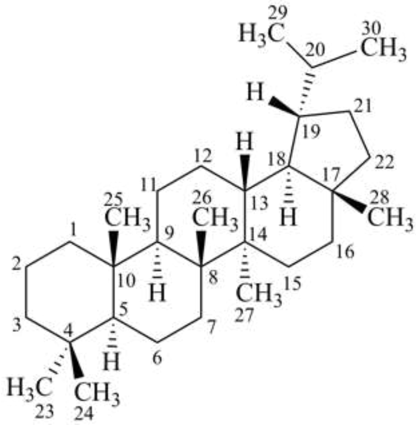


12
14
15
11
13
CH3
17
CH3
H
H
1
CH3
9
16
2
10
8
CH3
H
20
5
3
4
7
H
6
H3C
CH3
18
19

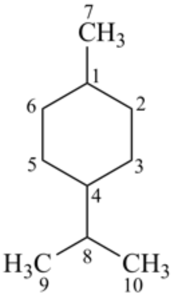
labdane
(named systematically by CAS)


H
21
H3C
22
24
26
CH3
18
CH3
20
23
25
12
H
11
17
CH3
27
19
13
CH3
H
16
1
9
14
2
10
8
H
CH3
30
3
5
7
4
H
6
H3C
28
CH3
29

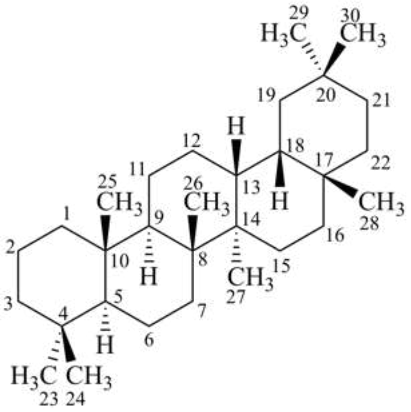
lanostane


29
H3C
20
30
CH3
H
21
19
H
12
22
11
18
17
25
CH3
26
CH3
13
H
28
CH3
1
9
14
16
2
10
8
H
CH3
27
15
3
5
7
4
H
6
H3C
23
CH3
24

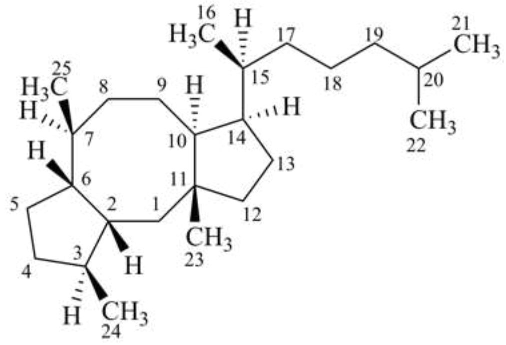
lupane


7
CH3
1
6
2
5
3
4
H3C
9
8
CH3
10

p-menthane
(named systematically by CAS)

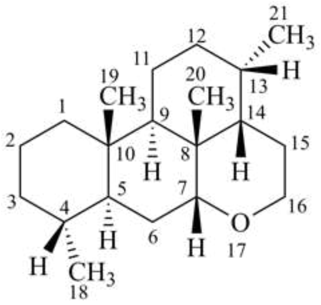

29
H3C
30
CH3
19
20
21
H
12
18
22
11
17
25
CH3
26
CH3
13
H
CH3
28
1
9
14
16
2
10
8
H
CH3
27
15
3
5
7
4
H
6
H3C
23
CH3
24

oleanane



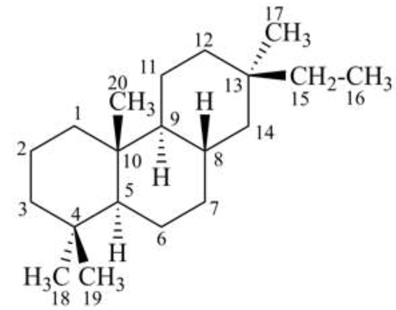
H_3C 16
H
15
17
18
19
20
21 CH_3
CH_3 22
H_3C 25
H
7
8
9
H
10
14
H
13
H
6
11
1
2
5
12
CH_3 23
3
4
H
H
CH_3 24

ophiobolane
(named systematically by CAS)



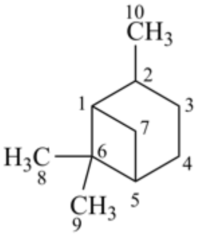
21 CH_3
12
11
H
13
19 CH_3
20 CH_3
1
9
8
14
2
10
H
H
15
3
4
5
7
O
16
H
H
6
17
H
CH_3 18

picrasane



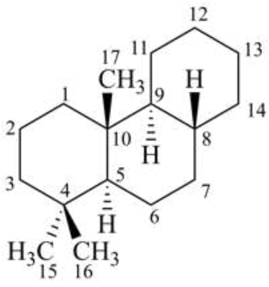
17 CH_3
12
11
13
CH_2-CH_3
15 16
20 CH_3
H
1
9
14
2
10
8
H
3
4
5
7
H
6
H_3C CH_3
18 19

pimarane
(named systematically by CAS)



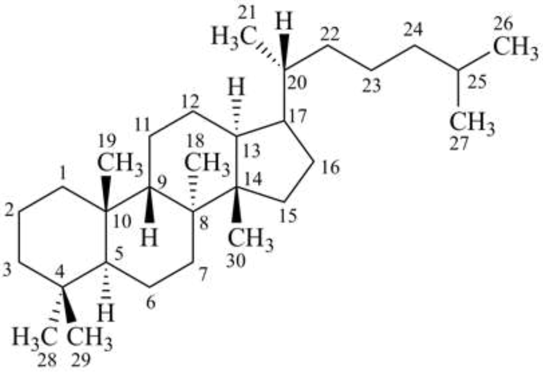
10 CH_3
2
1
3
7
H_3C
8
6
4
5
CH_3
9

pinane
(named systematically by CAS)

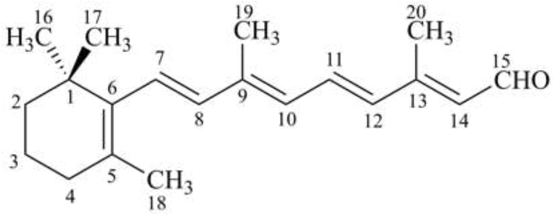


12
11
13
17 CH_3
H
1
9
14
2
10
8
H
3
4
5
7
H
6
H_3C CH_3
15 16

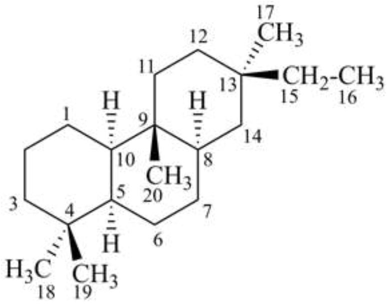
podocarpane
(named systematically by CAS)


H₃C
H
CH₃
CH₃
CH₃
CH₃
CH₃
H
H
H
H₃C CH₃
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30

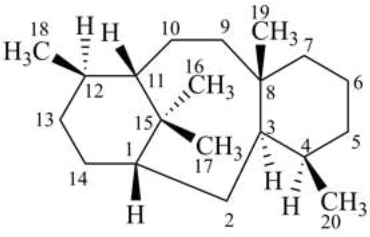
protostane
(named by CAS as a stereoisomer of dammarane)


H₃C
CH₃
CH₃
CH₃
CHO
CH₃
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20

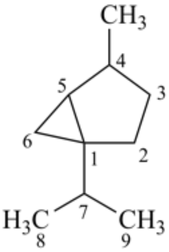
retinal


CH₃
CH₂-CH₃
H
H
CH₃
H
H₃C
CH₃
1 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20

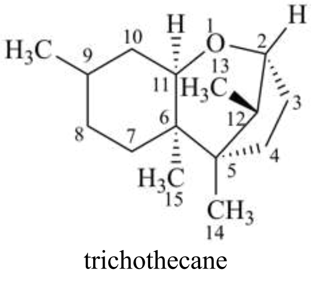
rosane
(named systematically by CAS)


H₃C
H
H
CH₃
CH₃
CH₃
H
H
H
CH₃
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20

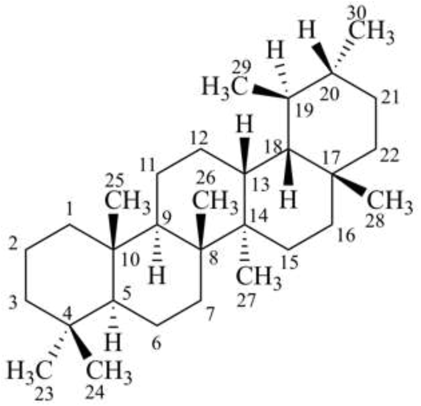
taxane
(named systematically by CAS)


CH₃
H₃C
CH₃
1 2 3 4 5 6 7 8 9

thujane
(named systematically by CAS)

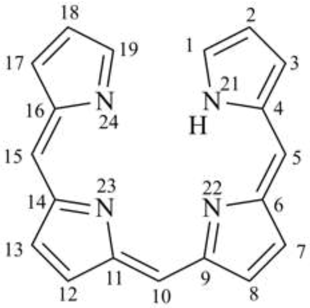

H₃C
H
O
H
H₃C
H₃C
CH₃
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15

trichothecane

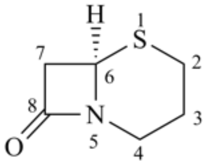

30
H
CH3
H
29
H3C
19
20
21
H
12
18
17
22
11
13
25
26
H
28
CH3
CH3
14
CH3
1
9
16
2
10
8
15
H
CH3
3
5
7
27
4
H
6
H3C
CH3
23
24

ursane

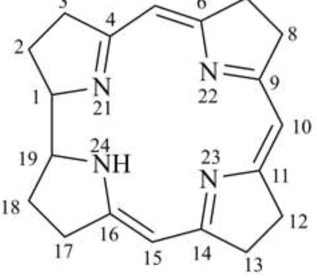
4. Miscellaneous


18
2
19
1
17
3
21
N
N
16
4
24
H
15
5
23
22
14
N
N
6
13
7
11
9
12
10
8

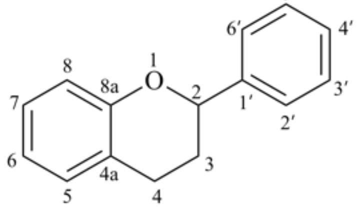
21*H*-biline


H
1
S
7
2
6
8
N
3
O
5
4

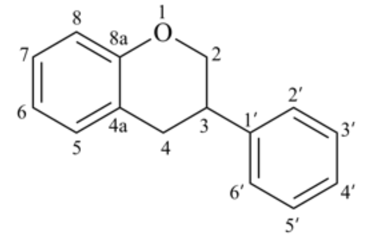
cepham
(named systematically by CAS)


3
5
7
4
6
8
2
N
N
9
1
21
22
10
24
23
19
NH
N
11
18
12
16
14
17
15
13

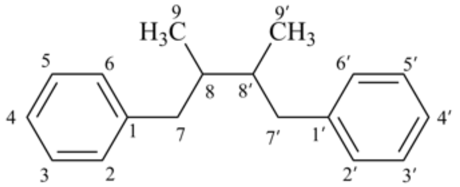
corrin


5′
6′
4′
1
8
O
8a
2
1′
3′
7
2′
6
3
4a
5
4

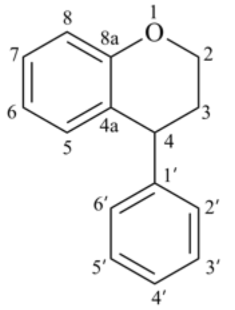
flavan
(named systematically by CAS)


O
1
2
3
4
4a
5
6
7
8
8a
1′
2′
3′
4′
5′
6′

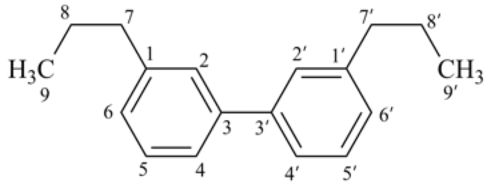
isoflavan
(named systematically by CAS)


H3C
9
CH3
9′
1
2
3
4
5
6
7
8
8′
7′
1′
2′
3′
4′
5′
6′

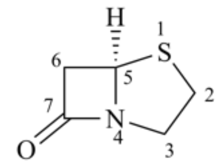
lignane
[only through a 8,8′ (β,β′) linkage]
(named systematically by CAS)


O
1
2
3
4
4a
5
6
7
8
8a
1′
2′
3′
4′
5′
6′

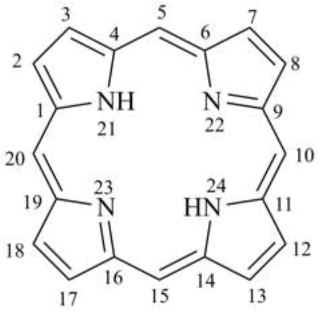
neoflavan
(named systematically by CAS)


H3C
9
8
7
1
2
3
4
5
6
3′
2′
1′
7′
8′
CH3
9′
6′
5′
4′

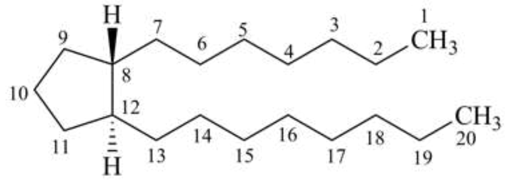
3,3′-neolignane
[and other structures not connected through a 8,8′) (β,β′) linkage]
(named systematically by CAS)


H
S
1
2
3
N
4
5
6
7
O

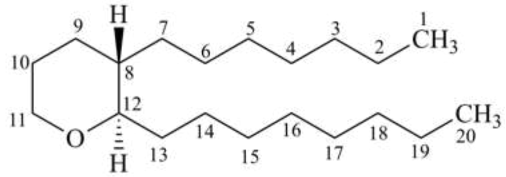
penam
(named systematically by CAS)


NH
21
N
22
N
23
HN
24
1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17
18
19
20

21*H*,23*H*-porphyrin
(named by CAS on the basis of the parent name porphine)



prostane



thromboxane
(named systematically by CAS)